

# **Heat Structure (HS) Package Reference Manual**

The MELCOR Heat Structure (HS) package calculates heat conduction within an intact, solid structure and energy transfer across its boundary surfaces. The modeling capabilities of heat structures are general and can include pressure vessel internals and walls, containment structures and walls, fuel rods with nuclear or electrical heating, steam generator tubes, piping walls, etc.

This document provides detailed information about the models, solution methods, and timestep control that are utilized by the HS package. Section 1 is an introduction to heat structure modeling and the calculation procedure. Section 2 provides details on the heat and mass transfer models. The solution methods utilized are discussed in Section 3, and timestep control is summarized in Section 4.

Information which is necessary to execute the HS package with other packages in the MELCOR code is found in the HS Users' Guide.

# HS Package Reference Manual

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## 1. Introduction

The Heat Structure (HS) package calculates heat conduction within an intact, solid structure and energy transfer across its boundary surfaces into control volumes. This document is the reference manual for the HS package. It contains the following information for this package:

- (1) detailed models,
- (2) solution methods, and
- (3) timestep control.

This section describes the modeling of a heat structure in the MELCOR code and provides a discussion of the calculation procedure which is used to obtain the temperature distribution and energy transfer for each heat structure and to calculate its interactions with structures in other packages.

A heat structure is an intact, solid structure which is represented by one-dimensional heat conduction with specified boundary conditions at each of its two boundary surfaces. The modeling capabilities of heat structures are general and can include pressure vessel internals and walls, containment structures and walls, fuel rods with nuclear or electrical heating, steam generator tubes, and piping walls.

Figure 1.1 illustrates a heat structure between two control volumes. A heat structure is inclined at some angle with respect to the vertical and is partially immersed. Although the geometry shown here is rectangular, a heat structure may have a rectangular, cylindrical, spherical, or hemispherical geometry.

The heat structure in Figure 1.1 is nodalized with  $N$  temperature nodes. The nodalization is specified by user input and may be nonuniform, i.e., the distance between temperature nodes need not be the same. Node 1 is the temperature node at the left boundary surface for a rectangular geometry or at the inside boundary surface for a cylindrical, spherical, or hemispherical geometry. Node  $N$  is the temperature node at the right boundary surface for a rectangular geometry or at the outside boundary surface for other geometries.

The region between two adjacent temperature nodes is called a mesh interval. Each mesh interval may contain a different material. The material in each mesh interval is specified by user input. The Material Properties package provides thermal properties for each material through an interface with the HS package. Most materials commonly found in PWRs and BWRs are included in the Material Properties package default database, and properties for materials which are not included can easily be defined through Materials Properties package user input (refer to the MP package documentation).

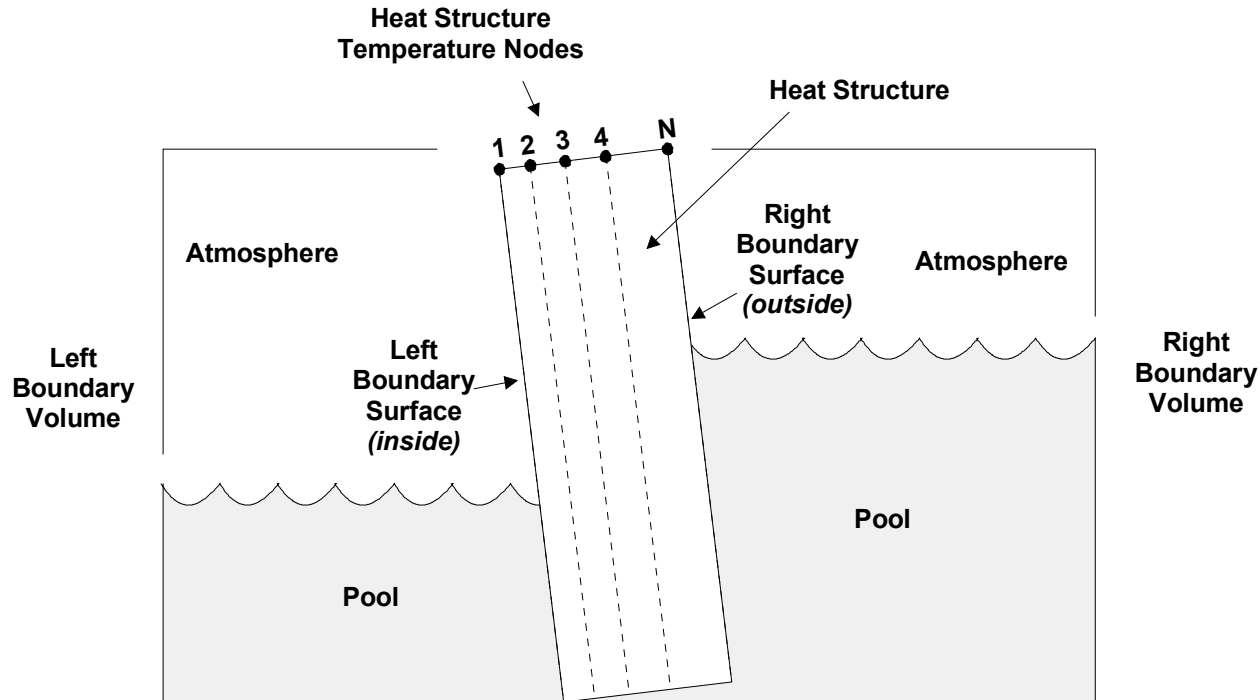


Figure 1.1 Heat Structure in a Control Volume

An internal power source may be specified for a heat structure. Its spatial dependence is specified by user input and may vary for each mesh interval. Its time dependence is given by a user-specified tabular function or control function.

Each heat structure has two boundary surfaces—left and right for rectangular geometries or inside and outside for cylindrical, spherical, or hemispherical geometries. At each boundary surface one of the following boundary conditions is specified:

- (1) symmetry (adiabatic)
- (2) convective with calculated heat transfer coefficient,
- (3) convective with calculated heat transfer coefficient and a specified surface power source function,
- (4) convective with specified heat transfer coefficient function,
- (5) specified surface temperature function, and
- (6) specified surface heat flux function.

If a convective boundary condition is selected for a boundary surface, a control volume must be specified as its boundary volume. Furthermore, the entire boundary surface must

fit within its boundary volume—that is, the bottom of the surface (user value HSALT) must equal or exceed the elevation of the bottom of the control volume specified in the CVH user input, and the top of the surface (calculated from HSALT and the surface length and orientation) must not exceed the elevation of the top of the control volume. No boundary volume is permitted for a symmetry or specified surface temperature boundary condition and a boundary volume for the specified heat flux boundary condition is a user option.

If a boundary volume is specified for a surface, then some additional data are required through user input. For each boundary surface with a boundary volume, these data are its

- (1) surface area,
- (2) characteristic length (the dimension used in calculating the Reynolds, Grashof, Nusselt, and Sherwood numbers),
- (3) axial length (length of structure along boundary surface, used to determine pool fraction),
- (4) type of flow over the surface (internal or external; used in calculating the Nusselt number), and
- (5) critical pool fractions for pool and atmosphere heat transfer.

The pool fraction of a heat structure boundary surface is the fraction of its surface area in the pool of its boundary volume. Pool fractions and critical pool fractions permit a weighting of heat and mass transfer to the boundary volume atmosphere and pool. These are discussed in detail in Section 2.4.

If a convective boundary condition with calculated heat transfer coefficient is specified, then an extensive set of correlations is available for calculating natural or forced convection to the pool and atmosphere. Pool boiling heat transfer is calculated if the temperature of a heat structure surface is above the boundary volume saturation temperatures by utilizing correlations for nucleate boiling, critical heat flux, film boiling, and transition boiling.

Radiation heat transfer from a heat structure surface to the boundary volume pool is calculated during boiling. Radiation heat transfer can also be specified between a heat structure surface and the boundary volume atmosphere. Note, however, that radiation heat transfer to the atmosphere will occur only if the atmosphere contains water vapor (steam) and/or carbon dioxide; all other gases are considered to be non-absorbing by MELCOR. Two options, an equivalent band model and a gray gas model, are currently available. Radiation between user-specified pairs of surfaces may also be modeled, as described in Section 2.6.2.2. Radiation heat transfer between the COR structures and HS structures is discussed in the COR package documentation.

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Mass transfer between a heat structure surface and the boundary volume atmosphere is modeled using correlations or expressions for calculating mass flux. Models include condensation and evaporation in the presence of noncondensibles with an appropriate limit for pure steam, and flashing in any environment. Liquid films on heat structure surfaces are also modeled so that condensate transferred from the boundary volume atmosphere and liquid deposited by other packages can be treated. An optional film tracking model is available to track condensate film drainage from structure to structure. The film tracking model is activated when the user defines one or more network(s) of connected structures, such as stacked cylindrical sections to represent the steam generator tubes and/or cylindrical shells capped by a hemisphere to represent a containment dome. The user also specifies a drainage pattern for each network, which consists of drainage destinations and fractions for the drainage from each structure in the network. Drainage from a structure surface may be partitioned between three destination types:

- (1) the surface of one or more additional structures in the network,
- (2) "rain" which is passed to the MELCOR Containment Sprays (SPR) package via the Transfer Process (TP) package, and/or
- (3) the pool of the CVH volume associated with the surface.

The user may also designate an external source of water for any structure in the network via tabular function input or a control function. External sources are primarily intended to allow the user to model the source for a passive containment cooling system or some such similar cooling device. When the film tracking model is active, the film thickness is calculated as a function of the condensate flow rate throughout the network.

Mass transfer affects the temperature distribution within a heat structure by its energy flux at the surface. This energy flux due to mass transfer is included in the boundary conditions for the conduction calculations, and film/atmosphere interfacial temperatures are calculated simultaneously with the structure node temperatures. The volume occupied by liquid films affects the virtual volume tracked by the CVH package, and the presence of liquid films also affects the rate and accumulation of radionuclides deposited on the surfaces by the RN package (see RN documentation). Decay heat from deposited radionuclides is treated as power source at the surface in the equation for the surface temperature.

Finite-difference equations are used to advance the temperature distribution of a heat structure in time during MELCOR execution or to obtain its steady-state temperature distribution during MELGEN execution if specified by user input. These equations are obtained from an integral form of the one-dimensional heat conduction equation and boundary condition equations utilizing a fully implicit numerical method. The finite-difference approximation is a tridiagonal system of  $N$  equations (or  $N + 1$  or  $N + 2$  if there is a liquid film on one or both surfaces of the structure) for a heat structure with  $N$  temperature nodes (or  $N + 1$  or  $N + 2$  temperature nodes if there is liquid film on one or



both surfaces of the structure). The solution of this system is obtained using the standard solution algorithm for a tridiagonal system of linear equations.

A degassing model is provided for the release of gases from materials which are contained in heat structure mesh intervals. Input may be provided, for example, to represent the release of water vapor or carbon dioxide from concrete as its temperature increases. The HS package calculates a constant gas release rate over the degassing temperature range and modifies the thermal properties over this range to account for the energy associated with the gas production and release. The degassing model is also used in a modified form to treat ice condensers.

Communication of mass and energy changes to other packages is achieved through well-defined interfaces.

The remainder of the reference manual amplifies this calculation procedure. An enumeration and description of all models employed in the HS package calculations are included in Section 2. The solution methods used by the HS package are discussed in Section 3. Section 4 elaborates on the timestep control use by this package.

The references for the HS Package Reference Manual are found in Section 5. Appendix A contains information on the sensitivity coefficients used in the HS package.

## **2. Detailed Models**

The modeling of a heat structure in the MELCOR Code System and the calculation procedure for the HS package are discussed in Section 1. This section provides a detailed description of the models that are utilized by the HS package in the calculation procedure.

Heat conduction within a heat structure is modeled by the heat conduction equation in one spatial dimension. This equation and the specification of boundary conditions constitute a well-defined mathematical problem for the temperature distribution of a heat structure. However, the generality of boundary conditions, the inclusion of surface power sources and mass transfer at each boundary surface, temperature-dependent thermal properties, spatial-dependent materials, and the variety of geometries preclude the possibility of analytic solutions for the temperature distribution. Therefore, the HS package utilizes numerical methods for the determination of the temperature distribution for each heat structure. The description of detailed models in the HS package begins in Section 2.1 with a presentation of the finite-difference equations that approximate the heat conduction equation within a heat source. The finite-difference equations that approximate the heat conduction equation at the boundary surfaces are presented in Section 2.2.

The finite-difference equations of Sections 2.1 and 2.2 require specification or calculation of the following:

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- (1) power sources,
- (2) pool fractions,
- (3) thermal properties,
- (4) heat transfer,
- (5) mass transfer, and
- (6) liquid film modeling.

Sections 2.3 through 2.8 provide the detailed models which specify these items.

Knowledge of the temperature distribution of a heat structure permits the calculation of its stored energy. The definition of stored energy of a heat structure is given in Section 2.9 within the context of the approximations of the HS package.

The thermal interactions between heat structures and control volumes result in the transfer of mass and energy between the CVH and HS packages. The HS package calculates such transfers between modules for the following:

- (1) heat flux,
- (2) liquid film evaporation and condensation, and
- (3) degassing.

The detailed modeling of these phenomena in the HS package is discussed in Sections 2.6, 2.7, and 2.10. The COR package calculates heat transfer from the core to the bounding heat structures and passes the resulting energy transfers to the appropriate heat structures through an interface with the HS package (see COR package documentation for further details).

### 2.1 Finite-Difference Equations for Interior

The equation that governs conduction heat transfer in the interior of a heat structure is the one-dimensional heat conduction equation. This equation has the form

$$C_p \frac{\partial T}{\partial t} = \frac{1}{A} \frac{\partial}{\partial x} \left( k A \frac{\partial T}{\partial x} \right) + U \quad (2.1)$$

where

$C_p$	= volumetric heat capacity (product of heat capacity at constant pressure and density)
$T$	= temperature
$\frac{\partial}{\partial t}$	= partial derivative with respect to time
$A$	= heat transfer area
$k$	= thermal conductivity
$\frac{\partial}{\partial x}$	= partial derivative with respect to spatial variable
$U$	= volumetric power

The heat conduction equation is a parabolic partial differential equation. The HS package must solve it with boundary and initial conditions to determine the temperature distribution at each point in a heat structure. Sections 2.1.1 and 2.1.2 discuss the finite-difference approximation of Equation (2.1) in the interior of a heat structure.

### 2.1.1 Nodalization at Interior Temperature Nodes

The finite-difference approximation of the heat conduction equation requires a spatial partitioning of the heat structure into a finite number of temperature nodes. Temperature nodes must be located at the boundary surfaces and at interfaces between different materials. Additional nodes may be located at arbitrary locations within individual materials.

The region between two adjacent temperature nodes is called a mesh interval. For rectangular geometries, the node locations are relative to the node at the left boundary; for cylindrical geometries, they are relative to the axis of the cylinder; and for spherical or hemispherical geometries, they are relative to the center of the sphere. The location of the temperature nodes increases in a monotonic manner from the node at the left or inside boundary surface.

Figure 2.1 illustrates the nodalization of the interior of a heat structure near the  $n$ -th temperature node. This figure contains three temperature nodes and the mesh intervals for which they are the boundary points. For a rectangular geometry, the HS volume which is depicted in Figure 2.1 is part of a rectangular solid; for a cylindrical geometry, it is part of a cylindrical shell; and for a spherical or hemispherical geometry, it is part of a spherical shell. The quantities represented in Figure 2.1 are:

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$N$	= number of temperature nodes in heat structure
$n$	= interior node number (2, 3, ..., N-1)
$X$	= location of temperature node
$\Delta X_n$	= $X_{n+1} - X_n$ , length of $n$ -th mesh interval
$k$	= thermal conductivity of material
$C_p$	= volumetric heat capacity of material
$U$	= volumetric power source

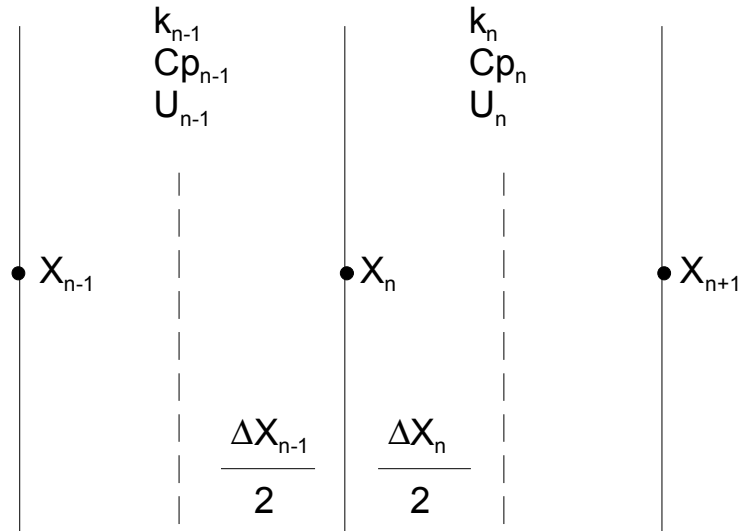


Figure 2.1 Nodalization in Interior of a Heat Structure

This figure also shows thermal properties and volumetric power sources in the mesh intervals adjacent to the  $n$ -th temperature node. These quantities are present in the finite-difference equations and are discussed in Sections 2.3 and 2.5.

To allow a more general representation of the equations and to consolidate expressions that define the numerical approximation, the following geometrical quantities are used [1]:

$HSL_n$	= left surface weight for $n$ -th temperature node
$HVL_n$	= left volume weight for $n$ -th temperature node
$HSR_n$	= right surface weight for $n$ -th temperature node

$HVR_n$  = right volume weight for  $n$ -th temperature node

Table 2.1 Surface and Volume Weights in Interior

Rectangular Geometries	Equation
$HSL_n = 1/\Delta X_{n-1}$	(2.2)
$HVL_n = \Delta X_{n-1}/2$	(2.3)
$HSR_n = 1/\Delta X_n$	(2.4)
$HVR_n = \Delta X_n/2$	(2.5)
Cylindrical Geometries	Equation
$HSL_n = 2\pi (X_n - \Delta X_{n-1}/2)/\Delta X_{n-1}$	(2.6)
$HVL_n = \pi [X_n^2 - (X_n - \Delta X_{n-1}/2)^2]$	(2.7)
$HSR_n = 2\pi (X_n + \Delta X_n/2)/\Delta X_n$	(2.8)
$HVR_n = \pi [(X_n + \Delta X_n/2)^2 - X_n^2]$	(2.9)
Spherical Geometries	Equation
$HSL_n = 4\pi (X_n - \Delta X_{n-1}/2)^2/\Delta X_{n-1}$	(2.10)
$HVL_n = (4\pi/3) [X_n^3 - (X_n - \Delta X_{n-1}/2)^3]$	(2.11)
$HSR_n = 4\pi (X_n + \Delta X_n/2)^2/\Delta X_n$	(2.12)
$HVR_n = (4\pi/3) [(X_n + \Delta X_n/2)^3 - X_n^3]$	(2.13)
Hemispherical Geometries	Equation
$HSL_n = 2\pi (X_n - \Delta X_{n-1}/2)^2/\Delta X_{n-1}$	(2.14)
$HVL_n = (2\pi/3) [X_n^3 - (X_n - \Delta X_{n-1}/2)^3]$	(2.15)

$HSR_n = 2\pi(X_n + \Delta X_n / 2)^2 / \Delta X_n$	(2.16)
$HVR_n = (2\pi/3) [(X_n + \Delta X_n / 2)^3 - X_n^3]$	(2.17)

The surface and volume weights in the interior of a heat structure are defined in Table 2.1. The interior temperature nodes correspond to  $n = 2, 3 \dots, N-1$ . The weights for  $n = 1$  and  $N$  are defined in Section 2.2.1.

The surface and volume weights may be interpreted by considering for each geometry the rectangular solids, cylindrical shells, and spherical shells which are bordered by a temperature node and have thicknesses equal to half the length of the mesh intervals adjacent to this node. For all geometries, each surface weight has a factor that is the reciprocal of the length of the appropriate mesh interval. These weights appear in the gradient terms of the difference equations. For rectangular geometries, the other factors in the surface weight and the volume weight are the surface area and volume per unit area of one of the solids, respectively. For cylindrical geometries, they are the surface area and volume per unit axial length of one of the shells; and for spherical or hemispherical geometries, they are the surface area and volume of one of the shells. By definition,  $HSL_{n+1} = HSR_n$  for all geometries, which ensures conservation.

### 2.1.2 Difference Approximation at Interior Nodes

The finite-difference equations are obtained from an integral form of the heat conduction equation. Consider multiplying Equation (2.1) by the area term and integrating the result over a heat structure. This integral equals the sum of integrals each of which is evaluated over a solid that is bounded by the dashed lines in Figure 2.1. The finite-difference approximation at the  $n$ -th interior temperature node is obtained from the integral of this equation over the solid that is bounded by these dashed lines. This approximation has the form

$$G_n (T_n^{m-1} - T_n^m) / \Delta t_m = k_{n-1} HSL_n (T_{n-1} - T_n) + k_n HSR_n (T_{n+1} - T_n) + (U_{n-1} HVL_n + U_n HVR_n) \quad (2.18)$$

where

$$\begin{aligned} T_n^m &= \text{temperature of } n\text{-th node at time } t_m \\ G_n &= Cp_{n-1} HVL_n + Cp_n HVR_n \\ U_n &= \text{volumetric power for } n\text{-th mesh interval} \end{aligned}$$

- $\Delta t_m$  = timestep for  $m$ -th computational cycle  
 $n$  = quantity at  $n$ -th temperature node or mesh interval  
 $m$  = quantity at time  $t_m$   
 $m+1$  = quantity at time  $t_m + \Delta t_m$

The time superscript for most of the terms in this equation is omitted. If all are  $m$ , then the finite-difference formulation is fully explicit. If all are  $m + 1$ , then the formulation is fully implicit. The fully implicit method is used by the HS package, so

$$G_n^{m+1} (T_n^{m+1} - T_n^m) / \Delta t_m = d_n^{m+1} \quad (2.19)$$

where

$$d_n^i = \text{right side of Equation (2.18) at time } t_i$$

For steady-state initialization calculations, the appropriate difference equation is

$$d_n = 0 \quad (2.20)$$

### 2.1.3 Finite-Difference Equations at Interior Temperature Nodes

The finite-difference equation at each interior temperature node is obtained by expanding Equation (2.19) or (2.20) and collecting the temperature terms at the  $m + 1$  time level on the left. This equation is

$$A_{n-1}^{m+1} T_{n-1}^{m+1} + B_n^{m+1} + C_n^{m+1} T_{n+1}^{m+1} = D_n^{m+1} \quad (2.21)$$

where, in addition to previously defined quantities,

$$A_n^{m+1} = -k_{n-1}^{m+1} HSL_n \Delta t_m$$

$$C_n^{m+1} = -K_n^{m+1} HSR_n \Delta t_m$$

$$B_n^{m+1} = A_n^{m+1} - C_n^{m+1} + a G_n^{m+1}$$

$$D_n^{m+1} = a G_n^{m+1} T_n^m + (U_{n-1}^{m+1/2} HVL_n + U_n^{m+1/2} HVR_n) \Delta t_m$$

$$\begin{aligned} a &= 1 \text{ for transient calculations} \\ &= 0 \text{ for steady-state calculations} \\ n &= 2, 3, \dots, N-1 \end{aligned}$$

The value of the power,  $U$ , is evaluated as the average of old and new time values in order to more accurately reflect the desired input energy. The result of applying Equation (2.21) to a heat structure with  $N$  temperature nodes is a tridiagonal system of  $N-2$  equations for the interior temperature nodes.

## 2.2 Finite-Difference Equations at Boundary Surfaces

The numerical calculation of the temperature distribution of a heat structure not only requires a finite-difference approximation of the heat conduction equation at interior temperature nodes, but also a finite-difference approximation of this equation and the boundary condition at each boundary surface.

There are two basic cases to consider at the surfaces of a structure:

- (1) the case when there is no liquid film on the surface, and
- (2) the case when there is a liquid film on the surface.

If there is no liquid film, then a boundary condition is applied to the structure surface and used to calculate the structure surface temperature. If a liquid film exists, then an additional mesh interval, consisting of the film bounded by the structure surface temperature node on the inside and the film/atmosphere interfacial temperature node on the outside, is defined, and a conduction equation for the film/atmosphere interfacial temperature is added to the set of  $N$  equations for the structure node temperatures. In this case, the equation for the structure surface (i.e., the structure/film interface) temperature is similar to the equations for the temperatures at the interior nodes, except that the half mesh interval on the outside consists of half of the liquid film instead of structure material. Hence, if there is no liquid film on either surface of the structure, the tridiagonal set will consist of  $N$  equations ( $N-2$  for interior nodes and 2 for the two surface node temperatures), while the set will consist of  $N+1$  (or  $N+2$ ) temperature equations, if there is a liquid film on one (or both) surfaces of the structure.

Only certain types of boundary conditions are permitted if mass transfer (liquid film condensation/evaporation) is to be treated; film formation is prohibited if an adiabatic, specified surface heat flux or specified surface temperature boundary condition is imposed.

**In the discussion that follows, it is to be understood that the boundary condition is applied at the film/atmosphere interface and not the structure/film interface if a liquid**



**film exists on the surface of the structure.** The general form of the boundary condition at the surface of a heat structure is

$$\alpha T + \beta \frac{dT}{dN} = \gamma \quad (2.22)$$

where

$\alpha$  = first boundary condition coefficient

$\beta$  = second boundary condition coefficient

$\gamma$  = third boundary condition coefficient

$T$  = temperature of surface

$\frac{dT}{dN}$  = gradient of temperature in direction of outward normal

This expression is implicit in the surface temperature, which is determined iteratively. All variables in this expression that are part of the heat structure package database (structure temperatures and properties that are functions of the structure temperature) are treated implicitly during the iteration procedure. Variables from other MELCOR packages (CVH temperatures and energy deposited by other packages) must be treated explicitly because of the explicit coupling between all MELCOR packages. All permitted boundary conditions can be put into this form as shown below.

## 2.2.1 Boundary Condition Coefficients

### 2.2.1.1 Symmetry (Adiabatic)

The symmetry boundary condition is represented by

$$\frac{dT}{dN} = 0 \quad (2.23)$$

For this boundary condition, the boundary condition coefficients are

$$\alpha = 0$$

$$\beta = 1$$

$$\gamma = 0$$

### 2.2.1.2 Convective (Calculated or Specified Heat Transfer Coefficients)

The convective boundary condition is represented by

$$-k \frac{dT}{dN} + S = (h_{atm} + h_{atmr})(1 - x_{pool})(T - T_{atm}) + h_{pool}x_{pool}(T - T_{pool}) \quad (2.24)$$

where

- $k$  = thermal conductivity
- $S$  = surface energy flux (flowing into heat structure)
- $h_{atm}$  = atmosphere heat transfer coefficient
- $h_{atmr}$  = atmosphere radiation heat transfer coefficient
- $x_{pool}$  = fraction of surface in pool of boundary volume
- $T_{atm}$  = temperature of atmosphere in boundary volume
- $h_{pool}$  = pool heat transfer coefficient
- $T_{pool}$  = temperature of pool in boundary volume

For these boundary conditions, the coefficients are

$$\begin{aligned} \alpha &= h_{pool}x_{pool} + (h_{atm} + h_{atmr})(1 - x_{pool}) \\ \beta &= k \\ \gamma &= h_{pool}x_{pool}T_{pool} + (h_{atm} + h_{atmr})(1 - x_{pool})T_{atm} + S \end{aligned}$$

### 2.2.1.3 Specified Surface Heat Flux

For specified heat flux at the surface, the boundary condition is represented by

$$-k \frac{dT}{dN} = q'' \quad (2.25)$$

where

$q''$  = specified heat flux at surface (positive out)

For these boundary conditions, the coefficients are

$$\alpha = 0$$

$$\beta = k$$

$$\gamma = -q''$$

#### 2.2.1.4 Specified Surface Temperature

The boundary condition for a specified surface temperature is represented by

$$T = T_{surf} = \text{specified surface temperature} \quad (2.26)$$

For these boundary conditions, the coefficients are

$$\alpha = 1$$

$$\beta = 0$$

$$\gamma = T_{surf}$$

### 2.2.2 Nodalization at Boundary Temperature Nodes

Figure 2.2 illustrates the geometry of a heat structure near the surface temperature nodes of a heat structure. This figure contains two temperature nodes and the mesh intervals for which they are the boundary points at both surfaces. It also depicts the condensate films which may or may not be present on each boundary surface. For all geometries, the volumes which are depicted in this figure are as described in Section 2.1.1. The quantities represented in Figure 2.2 are:

$N$  = number of temperature nodes in heat structure

$X$  = location of temperature node

$\Delta X_n$  =  $X_{n+1} - X_n$ , length of  $n$ -th mesh interval

$k$  = thermal conductivity of material

$c_p$  = volumetric heat capacity of material

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$U$	= volumetric power
$S$	= surface power
$\delta_f$	= thickness of liquid film
$m_f$	= mass of liquid film
$h_f$	= specific enthalpy of liquid film
$C_p$	specific heat of liquid film

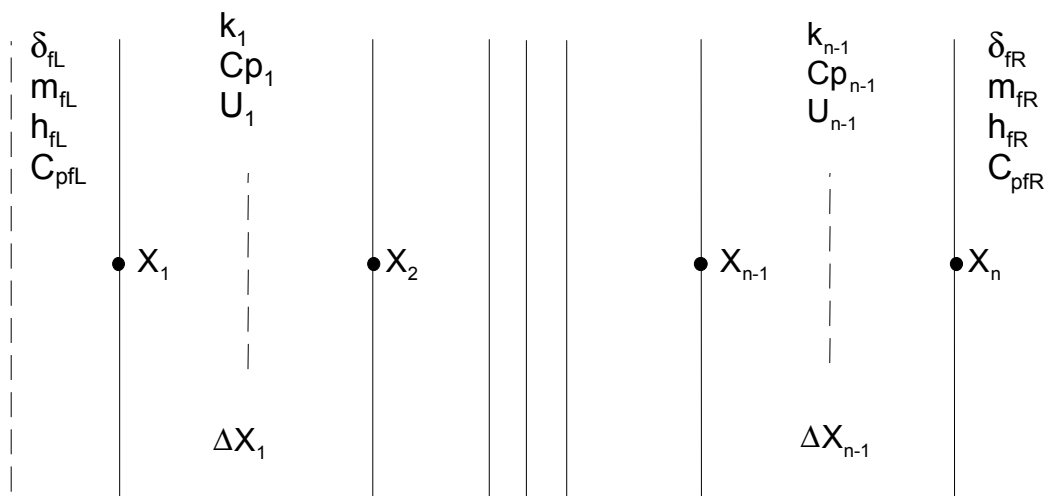


Figure 2.2 Nodalization at Boundary Surfaces of a Heat Structure

Table 2.2 Surface and Volume Weights at Boundary Surfaces

Rectangular Geometries	Equation
$HSL_1 = 1$	(2.27)
$HVL_1 = 0$	(2.28)
$HSR_1 = 1/\Delta X_1$	(2.29)
$HVR_1 = \Delta X_1/2$	(2.30)

$HSL_N = 1 / \Delta X_{N-1}$	(2.31)
$HVL_N = \Delta X_{N-1} / 2$	(2.32)
$HSR_N = 1$	(2.33)
$HVR_N = 0$	(2.34)
<b>Cylindrical Geometries</b>	<b>Equation</b>
$HSL_1 = 2\pi X_1$	(2.35)
$HVL_1 = 0$	(2.36)
$HSR_1 = 2\pi(X_1 + \Delta X_1 / 2) / \Delta X_1$	(2.37)
$HVR_1 = \pi[(X_1 + \Delta X_1 / 2)^2 - X_1^2]$	(2.38)
$HSL_N = 2\pi(X_N - \Delta X_{N-1} / 2) / \Delta X_{N-1}$	(2.39)
$HVL_N = \pi[X_N^2 - (X_N - \Delta X_{N-1} / 2)^2]$	(2.40)
$HSR_N = 2\pi X_N$	(2.41)
$HVR_N = 0$	(2.42)
<b>Spherical Geometries</b>	<b>Equation</b>
$HSL_1 = 4\pi X_1^2$	(2.43)
$HVL_1 = 0$	(2.44)
$HSR_1 = 4\pi(X_1 + \Delta X_1 / 2)^2 / \Delta X_1$	(2.45)
$HVR_1 = (4\pi / 3)[(X_1 + \Delta X_1 / 2)^3 - X_1^3]$	(2.46)
$HSL_N = 4\pi(X_N - \Delta X_{N-1} / 2)^2 / \Delta X_{N-1}$	(2.47)
$HVL_N = (4\pi / 3)[X_N^3 - (X_N - \Delta X_{N-1} / 2)^3]$	(2.48)

$HSR_N = 4\pi X_N^2$	(2.49)
$HVR_N = 0$	(2.50)
<b>Hemispherical Geometries</b>	<b>Equation</b>
$HSL_1 = 2\pi X_1^2$	(2.51)
$HVL_1 = 0$	(2.52)
$HSR_1 = 2\pi(X_1 + \Delta X_1/2)^2 / \Delta X_1$	(2.53)
$HVR_1 = (2\pi/3)[(X_1 + \Delta X_1/2)^3 - X_1^3]$	(2.54)
$HSL_N = 2\pi(X_N - \Delta X_{N-1}/2)^2 / \Delta X_{N-1}$	(2.55)
$HVL_N = (2\pi/3)[X_N^3 - (X_N - \Delta X_{N-1}/2)^3]$	(2.56)
$HSR_N = 2\pi X_N^2$	(2.57)
$HVR_N = 0$	(2.58)

The figure also shows thermal properties and volumetric power sources in the mesh intervals adjacent to the boundary nodes. These quantities are present in the finite-difference equations and are discussed in Sections 2.3 and 2.5.

The surface and volume weights are also defined at the boundary surfaces. The definitions are given in Table 2.2 for the case when no liquid film exists on either surface. The surface and volume weights for the case involving liquid films are similar, except there is one additional temperature node on each side that has a liquid film, and the mesh interval (with a thickness equal to that of the liquid film,  $\delta_f$ ) between the additional node (on the outside) and the structure surface node (on the inside) contains the liquid film. The surface and volume weights may be interpreted as discussed in Section 2.1.1 except (a) the left volume weight at the left (inside) temperature node and the right volume weight at the right (outside) temperature node are zero and (b) the left surface weight at the left (inside) temperature node and the right surface weight at the right (outside) boundary surface are the areas of these respective surfaces.

### 2.2.3 Difference Approximation at Boundary Nodes

The finite-difference equations at boundary nodes are obtained from an integral form of the heat conduction equation. The finite-difference approximation at the boundary temperature nodes is obtained from the integral of Equation (2.1) (multiplied by the area term) over the solid that is bounded by the film surface and the dashed line in Figure 2.2.

#### 2.2.3.1 Finite-Difference Equation at Left (Inside) Boundary

By using Equation (2.22) to eliminate the spatial derivative term, the finite-difference approximation has the following form at the left (inside) boundary surface:

$$G_1^{m+1}(T_1^{m+1} - T_1^m) / \Delta t_m = [k_1(y_L - \alpha_L T_1) / \beta_L] HSL_1 + k_1(T_2 - T_1) HSR_1 + U_1 HVR_1 - m_{f,L}^m \Delta h_{f,L} / f \quad (2.59)$$

If there is no liquid film on that surface (i.e., there was and is no film, or there was film that completely evaporated or was transferred to the pool associated with the boundary volume). If there is a liquid film, then the equations for the film surface temperature and structure surface temperature are:

$$G_{f,L}^{m+1}(T_{f,L}^{m+1} - T_{f,L}^m) / \Delta t_m = HSR_{f,L} H_{f,L} (T_1 - T_{f,L}) + HSL_{f,L} [(1 - x_{pool,L}) \cdot (H_{atm,L} + H_{atmr,L}) \cdot (T_{atm,L} - T_{f,L}) + x_{pool,L} H_{pool,L} \cdot (T_{pool,L} - T_{f,L})] + [(1 - x_{pool,L}) A_L / f] \cdot [(h_{V,L} - h_{f,L}) \cdot \max(0, \dot{m}_{C,L}) + (h_{V,L} - \bar{h}_{f,L}) \cdot \min(0, \dot{m}_{C,L})] \quad (2.60a)$$

$$(G_1^{m+1} + G_{f,L}^{m+1})(T_1^{m+1} - T_1^m) / \Delta t_m = HSR_1 k_1 (T_2 - T_1) - HSR_{f,L} H_{f,L} (T_1 - T_{f,L}) + [(1 - x_{pool,L}) A_L / f] (h_{f,L} - \bar{h}_{f,L}) \max(0, \dot{m}_{C,L}) + U_1 HVR_1 \quad (2.60b)$$

where

$$G_1^{m+1} = C_{p1}^{m+1} HVR_1$$

$f$  = geometry factor

= surface area of heat structure for rectangular geometries

= axial length of heat structure for cylindrical geometries

= 1.0 for spherical and hemispherical geometries

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$m_f^m$	= (old) mass of film evaporated (or transferred) this timestep
$\Delta h_f$	= specific enthalpy added to $m_f^m$ before its removal = latent heat of vaporization if film evaporated = 0.0 if film was transferred to pool
$HSR_f$	= HSR evaluated at film mass median surface
$HSL_f$	= HSL evaluated at film/atmosphere interface
$A$	= structure surface area
$x_{pool}$	= fraction of boundary surface in pool of boundary volume
$H_{atm}$	= convective heat transfer coefficient to atmosphere
$H_{atmr}$	= radiative heat transfer coefficient to atmosphere
$H_{pool}$	= convective heat transfer coefficient to pool
$H_f$	= convective/conductive heat transfer coefficient through film
$T_{atm}$	= temperature of atmosphere in boundary volume
$T_{pool}$	= temperature of pool in boundary volume
$m_f$	= mass of film
$\dot{m}_c$	= condensation/evaporation mass flux (+/- for cond/evap)
$c_{pf}$	= specific heat capacity of film
$G_f^{m+1}$	= $0.5 m_f^{m+1} c_{pf}^{m+1} / f$
$h_v$	= specific enthalpy of vapor in boundary volume
$h_{f,L}$	= specific enthalpy of film evaluated at film/atmosphere interfacial temperature
$h_{f,1}$	= specific enthalpy of film evaluated at structure/film interfacial temperature
$\bar{h}_f$	= $0.5 \times (h_{f,L} + h_{f,1})$



$L$	= quantity at left (inside) boundary surface
$i$	= quantity at $i$ -th temperature node or mesh interval
$m$	= quantity at time $t_m$
$m+1$	= quantity at time $t_m + \Delta t_m$

Equation (2.60) does not apply when  $\beta = 0$ . This corresponds to the specified surface temperature boundary condition, in which case  $T_1^{m+1} = T_{surf,L}^{m+1}$  and the presence of surface films and mass transfer is not permitted.

The time superscript for each term on the right side of Equation (2.60) is omitted. If all are  $m$ , then the finite-difference formulation is fully explicit. If all are  $m+1$ , then the formulation is fully implicit. The fully implicit numerical method is used by the HS package. Equation (2.60) is used for both steady-state (MELGEN) and transient (MELCOR) calculations, except that for steady-state calculations the old time values ( $m$ ) are overwritten with the new time values ( $m+1$ ) after each iteration. Hence, when convergence is achieved in MELGEN, temperatures that do not change with time (steady-state) have been determined. In MELGEN the timestep size is given by the value of sensitivity coefficient C4051(3), which is  $10^5$  s by default.

The finite-difference equation(s) at the left (inside) boundary temperature node(s) are obtained by expanding Equation (2.60) and collecting the temperature terms at the  $m+1$  time level on the left. Equation (2.60) reduces to

$$B_1^{m+1} T_1^{m+1} + C_1^{m+1} T_2^{m+1} = D_1^{m+1} \quad (2.61a)$$

where for  $\beta_L$  not zero,

$$\begin{aligned} B_1^{m+1} &= G_1^{m+1} - C_1^{m+1} + (\alpha_L^{m+1} k_1^{m+1} HSL_1 \Delta t_m) / \beta_L^{m+1} \\ C_1^{m+1} &= -k_1^{m+1} HSR_1 \Delta t_m \\ D_1^{m+1} &= G_1^{m+1} T_1^m + (\gamma_L^{m+1} k_1^{m+1} HSL_1 \Delta t_m) / \beta_L^{m+1} + U_1^{m+1/2} HVR_1 \Delta t_m \\ &\quad - m_{f,L}^m \Delta h_{f,L} / f \end{aligned}$$

and for  $\beta_L$  zero,

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$$B_1^{m+1} = 1$$

$$C_1^{m+1} = 0$$

$$D_1^{m+1} = \gamma_L^{m+1} = T_{surf,L}^{m+1}$$

Equation (2.60a) and (2.60b) reduce to

$$B_L^{m+1}T_L^{m+1} + C_L^{m+1}T_1^{m+1} = D_L^{m+1} \quad (2.61b)$$

$$A_1^{m+1}T_{f,L}^{m+1} + B_1^{m+1}T_1^{m+1} + C_1^{m+1}T_2^{m+1} = D_1^{m+1} \quad (2.61c)$$

where

$$B_L^{m+1} = G_{f,L}^{m+1} - C_L^{m+1} + HSL_{f,L} \left[ (1 - x_{pool,L}) (H_{atm,L}^{m+1} + H_{atmr,L}^{m+1}) + x_{pool,L} H_{pool,L}^{m+1} \right] \Delta t$$

$$C_L^{m+1} = -H_{f,L}^{m+1} HSR_{f,L} \Delta t_m$$

$$D_L^{m+1} = G_{f,L}^{m+1} T_{f,L}^m + HSL_{f,L} \left[ (1 - x_{pool,L}) (H_{atm,L}^{m+1} + H_{atmr,L}^{m+1}) T_{atm,L} + x_{pool,L} H_{pool,L}^{m+1} T_{pool,L} \right] \Delta t_m \\ + \left[ (1 - x_{pool,L}) A_L / f \right] \left[ (h_{v,L} - h_{f,L}^{m+1}) \max(0, \dot{m}_{c,L}^{m+1}) + (h_{v,L} - \bar{h}_{f,L}^{m+1}) \min(0, \dot{m}_{c,L}^{m+1}) \right] \Delta t_m$$

$$A_1^{m+1} = C_L^{m+1}$$

$$B_1^{m+1} = G_1^{m+1} + G_{f,L}^{m+1} - A_1^{m+1} - C_1^{m+1}$$

$$C_1^{m+1} = -k_1^{m+1} HSR_1 \Delta t_m$$

$$D_1^{m+1} = (G_1^{m+1} + G_{f,L}^{m+1}) T_1^m + \left[ (1 - x_{pool,L}) A_L / f \right] \left[ (h_{f,L}^{m+1} - \bar{h}_{f,L}^{m+1}) \max(0, \dot{m}_{c,L}^{m+1}) \right] \Delta t_m \\ + U_1^{m+1/2} HVR_1 \Delta t_m$$

### 2.2.3.2 Finite-Difference Equation at Right (Outside) Boundary

The finite-difference equation(s) at the right (outside) boundary surface are exactly analogous to those at the left (inside) boundary surface. The subscripts 1, 2 and L are merely replaced by subscripts N, N-1 and R; HSL and HSR are reversed; HVL and HVR are reversed; and matrix elements A and C are reversed.

## 2.3 Power Sources

Power sources are included in the calculation of the temperature distribution of each heat structure. These sources include the following:

- (1) internal power source,
- (2) surface power source, and
- (3) energy transferred by other packages.

These items are discussed in Sections 2.3.1 through 2.3.3, respectively.

### 2.3.1 Internal Power Sources

The internal power source is included in the temperature evolution equations as volumetric power terms in each mesh interval. User input specifies the spatial distribution of the power source for each heat structure that contains an internal power source. These data are used to calculate the fraction of power from a tabular function or control function that is applied to each mesh interval. The HS package calculates the volumetric power terms,  $U$ , that appear in the equations. For the  $n$ -th mesh interval,

$$U_n = x_{P,n} P_{\text{int}} / (HVL_{n+1} + HVR_n) / f \quad (2.62)$$

where

$n$  = 1,2,...,N-1

$N-1$  = number of mesh intervals

$x_P$  = fraction of power from tabular function that is applied to this mesh interval (user input)

$P_{\text{int}}$  = average of power from internal source tabular function at old and new times or power from a specified control function for transient calculations and time zero value for initialization calculations

$HVL$  = left (inside) volume weights defined in Sections 2.1.1 and 2.2.2

$HVR$  = right (outside) volume weights defined in Sections 2.1.1 and 2.2.2

$f$  = geometry factor with the following values for different geometries  
 = surface area of heat structure for rectangular geometries

= axial length of heat structure for cylindrical geometries

= 1.0 for spherical and hemispherical geometries

### 2.3.2 Surface Power Sources

For a convective boundary condition with calculated heat transfer coefficients, a surface power source may be specified by a user-input control function or a tabular function of time. This source is included in Equations (2.24) and (2.25) as energy fluxes which are added to the boundary condition coefficients,  $\gamma$ , in Equation (2.24). The HS package calculates these fluxes,  $q''_{surf}$ , prior to calculating the temperature distribution of each heat structure. For each boundary surface, these terms are

$$q''_{surf} = P_{surf} / A_{surf}$$

where

$q''_{surf}$  = energy flux at boundary surface from surface power source

$P_{surf}$  = average of surface power from tabular function at old and new times for transient calculations and zero for initialization calculations

$A_{surf}$  = area of boundary surface

### 2.3.3 Energy Transferred by Other Packages

The energy which is transferred to a heat structure surface by other packages is obtained from an array in the HS package data base whose elements are updated using an interface subroutine that can be called any package. This energy includes, for example, the radiant energy from a core cell, conduction from debris deposited on the structure surface by the high-pressure-melt-ejection (HPME) model of the FDI package or the decay-heat energy of radionuclides deposited on a heat structure surface. This energy is included in Equations (2.24) and (2.25) as energy fluxes which are added to the boundary condition coefficients  $\gamma$  in Equation (2.24). The HS package calculates these fluxes,  $q''_{ext}$ , prior to calculating the temperature distribution of each heat structure. For each boundary surface, these terms are

$$q''_{ext} = E_{ext} / A_{surf} / \Delta t \quad (2.63)$$

where

$q''_{ext}$  = energy flux at boundary surface from energy which is transferred by other packages

$E_{ext}$  = energy which is transferred to boundary surface by other packages since the previous call to the HS package for transient calculations and zero for initialization calculations

$A_{surf}$  = area of boundary surface

$\Delta t$  = computational timestep

For each boundary surface, the surface energy flux term  $S$  in Equation (2.24) used in determining the boundary coefficient  $\gamma$  is the sum of  $q''_{surf}$  and  $q''_{ext}$  obtained from the above equations.

## 2.4 Pool Fractions

When a heat structure with a convective boundary condition is in contact with a CVH volume containing either single-phase liquid or vapor, the implementation of the boundary condition is straightforward. However, if the surface is partially submerged, then it is necessary to partition the heat transfer between the pool and the atmosphere as described in Section 2.2.1.2. In this case, heat transfer is partitioned on the basis of a calculated fraction of the heat structure surface that is submerged as depicted in Figure 1.1. This fraction is called the pool fraction with a range of 0 to 1. This section describes how the pool fraction is calculated for each type of geometry and the controls available to the user.

There are two input parameters for each surface, CPFPL and CPFAL, which allow the user to disable heat transfer to the pool and/or atmosphere as a function of the pool fraction. The range of each is 0 to 1. Heat transfer to the pool is calculated only when the pool fraction exceeds the critical pool fraction CPFPL. Similarly, heat and mass transfer to the atmosphere occur only when the pool fraction falls below the critical pool fraction CPFAL. Note that CPFPL and CPFAL are completely independent. Furthermore, disabling heat transfer to either phase will not affect heat transfer to the other phase directly. Also, when permitted, the heat transfer rates are independent of the values of CPFPL and CPFAL. When heat transfer from either phase is permitted, it occurs over the fraction of the surface area that is in contact with that phase (as given by  $x_{pool}$  for the pool and  $1-x_{pool}$  for the atmosphere in Equation (2.24)). When heat transfer to either phase is disabled it is as though there is a perfectly insulating layer at the interface.

The primary use of this input feature is to prohibit simultaneous heat transfer to both pool and atmosphere when such an occurrence will generate unrealistic results. The most common situation to be avoided occurs when a vertical structure is in contact with both a cool liquid pool and a hot atmosphere. In this case, if the heat structure is allowed to

communicate with both phases simultaneously, the relatively large heat transfer coefficient to the pool pulls the one-dimensional structure surface temperature down to a value much closer to the pool temperature than the atmosphere temperature. Consequently, heat transfer from the atmosphere to the structure is much greater than should be expected. The net effect is an artificially large heat transfer from the atmosphere to the pool via the structure surface. This situation can be avoided by specifying equal values of CPFPL and CPFAL so that structure only communicates to either the pool or atmosphere.

For situations in which the pool and atmosphere temperatures in the boundary control volume are nearly the same and heat transfer to both phases is expected to be significant, the user should enable simultaneous communications with both phases by specifying a value of zero for CPFPL and one for CPFAL. This option is often used for steam generator heat structures. This should also be used for horizontal floors and ceiling for which the pool fraction is specially modified as described in Section 2.4.1.

A value of 0.0 for CPFPL, or of 1.0 for CPFAL, can lead to numerical problems because heat transfer may be calculated to an arbitrarily small fluid mass if the heat structure extends to the bottom or top of the control volume, respectively. To avoid this potential problem, bounds are imposed on the user-input values so that  $CPFPL \geq 0.02$  and  $CPFAL \leq 0.98$ . These bounds are contained in sensitivity coefficient array 4071.

If CPFPL is greater than CPFAL, there will be a dead band with no communication to either the pool or atmosphere. This unlikely situation is not currently treated as a fatal input error.

If CPFPL is less than CPFAL, there will be a band with simultaneous heat transfer to both pool and atmosphere.

If CPFPL is equal to CPFAL, heat transfer will switch from one phase to the other as the pool fraction crosses the critical value. In the special case where the calculated pool fraction is exactly equal to the common value of CPFPL and CPFAL, communication will be to the pool if the value is greater than or equal to 0.5 and to the atmosphere otherwise.

Because of the potential for serious problems when unequal values of CPFPL and CPFAL are specified, MELGEN will generate a warning message to alert the user to the potential for unrealistic results. Nevertheless, if simultaneous heat transfer to both the pool and atmosphere is unlikely to cause serious problems, then CPFPL and CPFAL should be chosen to permit simultaneous heat transfer (i.e., set  $CPFPL = 0$  and  $CPFAL = 1$ ).

The pool fraction for a surface is set to 0.0 if its lowest point is above the pool and set to 1.0 if it is completely immersed in the pool. If the pool/atmosphere interface is very close to the top or bottom of a heat structure surface (less than the maximum film thickness), the pool fraction is set to 1.0 or 0.0, respectively. For all other situations, the expressions given below are evaluated for the pool fraction. Sections 2.4.1 through 2.4.4 present these expressions for rectangular, cylindrical, spherical, and hemispherical geometries, respectively.

### 2.4.1 Rectangular Geometry

The pool fraction for a surface with a rectangular geometry is given by

$$x_{pool} = Z / L \cos(\alpha) \quad (2.64)$$

where

- $Z$  = depth of pool in boundary volume of this surface relative to the altitude of the lowest point on this surface
- $L$  = axial length of this surface
- $\alpha$  = angle between this surface and the vertical

For horizontal surfaces, such as floors and ceilings, where  $\cos(\alpha) = 0$  in Equation (2.64), the pool fraction is defined to vary from zero to one as the pool surface ascends through a vertical distance of the maximum of liquid film thickness (see Section 2.8) and  $10^{-6}$  m, which eliminates a step change in pool fraction.

### 2.4.2 Cylindrical Geometry

The following quantities are used for defining the pool fraction for a surface with a cylindrical geometry:

- $R$  = radius of cylinder containing the surface
- $L$  = axial length of this surface
- $\alpha$  = angle between this surface and the vertical
- $a$  = vertical projection of cylinder diameter,  $2R \sin(\alpha)$
- $b$  = vertical projection of cylinder axial length,  $L \cos(\alpha)$
- $Z$  = depth of pool in boundary volume of this surface relative to the altitude of the lowest point on this surface

The pool fraction for a vertical surface,  $\cos(\alpha)=1$ , with a cylindrical geometry is given by

$$x_{pool} = Z / L \quad (2.65)$$

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The pool fraction for a horizontal surface,  $\cos(\alpha)=0$ , with a cylindrical geometry is given by

$$X_{pool} = \Theta / \pi \quad (2.66)$$

where

$$\Theta = \cos^{-1}[(R - Z)/R],$$

is in radians and is  $\pi$  for  $Z > 2R$ .

The pool fraction for a cylinder inclined at an angle  $\alpha$  between vertical and horizontal is given as follows:

$$X_{pool} = R \sin(\alpha) [TERML(Z) + TERM(R(Z))] / b \quad (2.67)$$

where  $TERML(Z)$  and  $TERM(R(Z))$  are functions of  $Z$  that are derived by considering whether or not the pool surface intersects the bottom and/or top flat surfaces of the cylinder. Defining

$$XL = 1 - Z / [R \sin(\alpha)] \quad (2.68)$$

it can be shown that, if the pool intersects the bottom surface ( $XL > -1$ ), then

$$TERML = \frac{1}{\pi} \left\{ [1 - XL^2]^{1/2} - \frac{XL}{\cos(XL)} \right\} \quad (2.69)$$

Otherwise, the bottom surface is completely submerged, and

$$TERML = -XL \quad (2.70)$$

Similarly, defining

$$XU = (a + b - z) / [R \sin(\alpha)] - 1 \quad (2.71)$$

It can be shown that



$$TERMR = \frac{1}{\pi} \left\{ \frac{XU}{\cos(XU)} - [1 - XU^2]^{1/2} \right\} \quad (2.72)$$

when the surface intersects the top end ( $XU < 1$ ); otherwise,

$$TERMR = 0 \quad (2.73)$$

### 2.4.3 Spherical Geometry

The pool fraction for a surface with a spherical geometry is given by

$$x_{pool} = Z / 2R \quad (2.74)$$

### 2.4.4 Hemispherical Geometry

The pool fraction for a surface with a hemispherical geometry is given by

$$x_{pool} = Z / R \quad (2.75)$$

## 2.5 Thermal Properties

The conduction equations require the thermal conductivity and volumetric heat capacity (product of heat capacity and density) of the material in each mesh interval. These thermal properties are discussed in Section 2.5.1. Their modification for a degassible material is discussed in Section 2.5.2.

### 2.5.1 Thermal Conductivity and Volumetric Heat Capacity

The thermal conductivity, heat capacity, and density of the material in each mesh interval are obtained as a function of temperature using an interface with the Material Properties package. They are obtained for the material in each mesh interval at a temperature that is the average of the temperatures of the nodes which are boundaries of this mesh interval.

### 2.5.2 Modifications for Degassible Materials

The volumetric heat capacity of a degassible material whose temperature is in the degassing temperature range is increased by an amount equal to the product of the heat of reaction and the source density divided by the degassing temperature range. The volumetric heat capacity is therefore replaced by

$$C_p + \Delta h_R \rho_{gas} / \Delta T_{gas} \quad (2.76)$$

where

$C_p$  = volumetric heat capacity from Material Properties package, kJ/m<sup>3</sup>•K

$\Delta h_R$  = heat of reaction of gas source, kJ/kg

$\rho_{gas}$  = density of gas in source, kg/m<sup>3</sup>

$\Delta T_{gas}$  = degassing temperature range of gas source, K

This modification accounts for the energy which is required to produce and release the gas.

## 2.6 Heat Transfer

The methods of calculating heat transfer at a heat structure surface are discussed in this section for the following:

- (1) specified temperature boundary conditions
- (2) specified heat flux boundary conditions
- (3) convective boundary conditions

If the temperature of a surface is specified by a tabular function, the heat flux is calculated from a finite-difference approximation which expresses the surface heat flux in terms of temperatures at the surface and adjacent nodes and quantities known in the interior of the heat structure. For the left boundary surface, this heat flux is given by

$$q_L'' = \left[ -k_1^{m+1} (T_1^{m+1} - T_2^{m+1}) HSR_1 + U_1 HVR_1 - Cp_1^m \frac{T_1^{m+1} - T_1^m}{\Delta t_m} HVR_1 \right] / HSL_1 \quad (2.77)$$

For the right boundary surface, this heat flux is

$$q_R'' = \left[ -k_N^{m+1} (T_N^{m+1} - T_{N-1}^{m+1}) HSL_N + U_N HVL_N - Cp_N^m \frac{T_N^{m+1} - T_N^m}{\Delta t_m} HVL_N \right] / HSR_1 \quad (2.78)$$

where

$k^m$	= thermal conductivity of heat structure at time $t_m$
$C_p^m$	= volumetric heat capacity of heat structure at time $t_m$
$HSL$	= left (inside) surface weight defined in Section 2.2.1
$HSR$	= right (outside) surface weight defined in Section 2.2.1
$HVL$	= left (inside) volume weight defined in Section 2.2.1
$HVR$	= right (outside) volume weight defined in Section 2.2.1
$U^m$	= volumetric power source at time $t_m$
$T^m$	= node temperature at time $t_m$
$T^{m+1}$	= node temperature at time $t_{m+1}$
$\Delta t$	= timestep size, $t_{m+1} - t_m$

If the surface heat flux is specified by a tabular function, the heat flux is known from the value of the tabular function.

If a convective boundary condition is specified, the heat flux is the product of the heat transfer coefficient and the temperature difference between the surface (film surface, if a liquid film is present) and the atmosphere or pool of the boundary volume. The heat transfer coefficient is either calculated or provided by a tabular function of time or temperature.

If a convective boundary condition with calculated heat transfer coefficients is specified, then correlations are available for the following heat transfer regimes:

- (1) atmosphere natural convection
- (2) atmosphere forced convection
- (3) pool natural convection
- (4) pool forced convection
- (5) pool boiling

The HS package calculates convective heat transfer between a heat structure and the boundary volume atmosphere whenever the pool fraction at a boundary surface is less than or equal to its critical pool fraction for atmosphere heat transfer. Atmosphere heat transfer occurs through a gas boundary layer and, if condensate is present on the surface,

through a liquid layer between the surface and the boundary layer. Radiation heat transfer also can occur between a heat structure and the boundary volume atmosphere. For this case, radiation and convection for the structure surface (or the film surface, if a liquid film exists) occur in parallel with one another (and in series with conduction/convection through the liquid film to the structure surface).

Heat transfer through the gas boundary layer is accounted for by a heat transfer coefficient obtained from correlations for natural or forced convection heat transfer. User input must specify whether an internal flow or external flow correlation is to be used when calculating atmosphere heat transfer coefficients for each boundary surface. These correlations are given in Section 2.6.1 for atmosphere heat transfer. Section 2.6.1.1 describes the modeling of heat transfer through liquid films when the film tracking model is inactive. The modeling of heat transfer through liquid films flowing over structures included in user-defined film tracking networks is discussed in Section 2.6.1.2.

Radiation heat transfer between a heat structure surface and the boundary volume atmosphere is modeled in either of two ways. The user has the option of employing the equivalent band model or the gray gas model for radiation heat transfer. These models are presented in Section 2.6.2.

At any surface, an arbitrary, user-specified nonnegative scaling factor may be applied to the calculated convective and radiative heat transfer coefficients to the atmosphere. The user may also apply a separate, arbitrary nonnegative scaling factor to the condensation/evaporation mass transfer coefficient. Users are cautioned that the application of significantly different heat and mass transfer scaling factors at the same surface may lead to nonphysical results and numerical problems. The scaling factors are provided primarily for conducting sensitivity studies associated with uncertainties related to surface fouling, local fluid effects, etc.

The HS package calculates heat transfer between a heat structure and the boundary volume pool whenever the pool fraction at a boundary surface is greater than or equal to its critical pool fraction for pool heat transfer. Pool heat transfer can be by natural convection, forced convection, or pool boiling. The HS package uses an extensive set of correlations for natural or forced convection pool heat transfer. User input must again specify whether an internal flow or external flow correlation is to be used when calculating pool heat transfer coefficients for each boundary surface. These correlations are exhibited in Section 2.6.3.

Pool boiling heat transfer is calculated at a surface if its pool fraction is greater than the critical pool fraction and its temperature is greater than the saturation temperature of its boundary volume (at total pressure). In calculating pool boiling heat transfer, the HS package uses a set of correlations for nucleate boiling, critical heat flux, minimum film boiling, and stable film boiling. Radiation heat transfer between a surface and the pool of its boundary volume is calculated during stable film and transition boiling. Correlations for

pool boiling heat transfer as well as models for pool radiation heat transfer are discussed in Section 2.6.4.

The HS package obtains the boiling heat transfer coefficient at a boundary surface as the quotient of the boiling heat flux and the difference between the temperature of this surface and the saturation temperature of its boundary volume (at total pressure).

The correlation of experimental heat transfer data is usually accomplished with dimensionless variables which are obtained by dimensional analysis or physical reasoning. These variables include:

$$\text{Reynolds number (Re)} = \rho V L_c / \mu$$

$$\text{Prandtl number (Pr)} = \mu c_p / k$$

$$\text{Grashof number (Gr)} = g \beta \Delta t L_c^3 \rho^2 / \mu^2$$

$$g |\rho_{srf} - \rho| L_c^3 \rho / \mu^2 \text{ (during condensation)}$$

$$\text{Nusselt number (Nu)} = h L_c / k$$

$$\text{Rayleigh number (Ra)} = Gr \cdot Pr$$

where

$$\rho = \text{density of atmosphere (pool), kg/m}^3$$

$$\rho_{srf} = \text{density of atmosphere evaluated at film surface temperature}$$

$$V = \text{velocity of atmosphere (pool), m/s}$$

$$L_c = \text{characteristic length of surface, m}$$

$$\mu = \text{viscosity of atmosphere (pool), kg/m}\cdot\text{s}$$

$$c_p = \text{heat capacity at constant pressure of atmosphere (pool), J/kg}\cdot\text{K}$$

$$k = \text{thermal conductivity of atmosphere (pool), W/m}\cdot\text{K}$$

$$g = \text{acceleration of gravity, m/s}^2$$

$$\beta = \text{volume coefficient of expansion of atmosphere (pool), K}^{-1}$$

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$\Delta t$  = magnitude of difference between temperatures of surface and atmosphere (pool), K

$h$  = atmosphere (pool) heat transfer coefficient, W/m<sup>2</sup>•K

The HS package uses these variables for selecting the appropriate heat transfer correlation or in expressing the functional form of the correlation for all heat transfer regimes except pool boiling. The pool boiling correlations are not expressed in a dimensionless form.

### 2.6.1 Atmosphere Convection Heat Transfer

Natural, forced, or mixed convection heat transfer to the atmosphere is determined at a surface by the following criteria:

Region	Criteria	Equation
Natural Convection	$Re^2 < 1.0 Gr$	(2.79)
Forced Convection	$Re^2 > 10.0 Gr$	(2.80)
Mixed Convection	$1.0 Gr \leq Re^2 \leq 10.0 Gr$	(2.81)

where

$Re$  = Reynolds number for atmosphere

$Gr$  = Grashof number for atmosphere

$Ra$  = Rayleigh number for atmosphere

The constants in Equations (2.79) through (2.81) are implemented as sensitivity coefficient array C4060.

The atmosphere natural convection heat transfer correlations have the following form:

$$Nu = C Ra^m + D \quad (2.82)$$

where

$Nu$  = Nusselt number

$Ra$  = Rayleigh number

$C, m, D$  = constants dependent on flow condition and geometry

The constants  $C$ ,  $m$ , and  $D$  in Equation (2.82) have been implemented as sensitivity coefficient arrays C4101 – C4112 and are presented in Table 2.3 for the various flow conditions and geometries.

Table 2.3 Constants for HS Package Heat Transfer Correlations

Region	Type of Flow		Geometry	(1)	(2)	(3)	(4)	Ref	SC Array	
ATMOSPHERE										
ATMOSPHERE	Natural Convection	Internal	Laminar	Rectangular	0.046	1/3	0	-	[1]	C4101
				Cylindrical	0.046	1/3	0	-	[1]	C4102
				Spherical	0.228	0.226	0	-	[1]	C4103
		Turbulent	Rectangular	0.046	1/3	0	-	[1]	C4104	
			Cylindrical	0.046	1/3	0	-	[1]	C4105	
			Spherical	0.228	0.226	0	-	[1]	C4106	
	Atmosphere	External	Laminar	Rectangular	0.59	0.25	0	-	[1]	C4107
				Cylindrical	0.59	0.25	0	-	[1]	C4108
				Spherical	0.43	0.25	2.0	-	[1]	C4109
		Turbulent	Rectangular	0.10	1/3	0	-	[1]	C4110	
			Cylindrical	0.10	1/3	0	-	[1]	C4111	
			Spherical	0.43	0.25	2.0	-	[1]	C4112	
ATMOSPHERE	Forced Convection	Internal	Laminar	Rectangular	8.235	0	0	0	[1]	C4113
				Cylindrical	48/11	0	0	0	[1]	C4114
				Spherical	48/11	0	0	0	[1]	C4115
		Turbulent	Rectangular	0.023	0.8	1/3	0	[2]	C4116	
			Cylindrical	0.023	0.8	1/3	0	[2]	C4117	
			Spherical	0.023	0.8	1/3	0	[2]	C4118	
	Pool	External	Laminar	Rectangular	0.664	0.5	1/3	0	[2]	C4119
				Cylindrical	0.664	0.5	1/3	0	[2]	C4120
				Spherical	0.60	0.5	1/3	2.0	[2]	C4121
		Turbulent	Rectangular	0.037	0.8	1/3	0	[2]	C4122	
			Cylindrical	0.037	0.8	1/3	0	[2]	C4123	
			Spherical	0.60	0.5	1/3	2.0	[2]	C4124	
POOL										
POOL	Natural Convection	Internal	Laminar	Rectangular	0.046	1/3	0	-	[1]	C4151
				Cylindrical	0.046	1/3	0	-	[1]	C4152
				Spherical	0.028	0.226	0	-	[1]	C4153
		Turbulent	Rectangular	0.046	1/3	0	-	[1]	C4154	
			Cylindrical	0.046	1/3	0	-	[1]	C4155	
			Spherical	0.228	0.226	0	-	[1]	C4156	
	Pool	External	Laminar	Rectangular	0.59	0.25	0	-	[1]	C4157
				Cylindrical	0.59	0.25	0	-	[1]	C4158
				Spherical	0.43	0.25	2.0	-	[1]	C4159
		Turbulent	Rectangular	0.10	1/3	0	-	[1]	C4160	
			Cylindrical	0.10	1/3	0	-	[1]	C4161	
			Spherical	0.43	0.25	2.0	-	[1]	C4162	
		Rectangular	8.235	0	0	0	[1]	C4163		

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Region	Type of Flow	Geometry	(1)	(2)	(3)	(4)	Ref	SC Array	
Forced Convection	Internal	Laminar	Cylindrical	48/11	0	0	0	[1]	C4164
			Spherical	48/11	0	0	0	[1]	C4165
		Turbulent	Rectangular	0.023	0.8	1/3	0	[2]	C4166
			Cylindrical	0.023	0.8	1/3	0	[2]	C4167
			Spherical	0.023	0.8	1/3	0	[2]	C4168
	External	Laminar	Rectangular	0.664	0.5	1/3	0	[2]	C4169
			Cylindrical	0.664	0.5	1/3	0	[2]	C4170
			Spherical	0.60	0.5	1/3	2.0	[2]	C4171
		Turbulent	Rectangular	0.037	0.8	1/3	0	[2]	C4172
			Cylindrical	0.037	0.8	1/3	0	[2]	C4173
			Spherical	0.60	0.5	1/3	2.0	[2]	C4174

The atmosphere forced convection heat transfer correlations have the following form:

$$Nu = C Re^m Pr^n + D \quad (2.83)$$

where

$Nu$  = Nusselt number

$Re$  = Reynolds number

$Pr$  = Prandtl number

$C, m, n, D$  = constants dependent on flow condition and geometry

The constants  $C$ ,  $m$ ,  $n$ , and  $D$  in Equation (2.83) have been implemented as sensitivity coefficient arrays C4113 – C4124 and are presented in Table 2.3 for the various flow conditions and geometries.

The Nusselt number in the mixed convection regime is a linear interpolation between the Nusselt numbers for the natural and forced convection regimes, based on the ratio  $Re^2/Gr$ . That is,

$$Nu_{mixed} = \left[ (Re^2/Gr - 1)/9 \right] [Nu_{forced} - Nu_{natural}] + Nu_{natural} \quad (2.84)$$

The constants in Equation (2.84) are, of course, derived from the sensitivity coefficients that define the limits of natural and forced convection. If the values of these coefficients do not define a proper transition—specifically if the upper limit for natural convection, C4060(1) (default value 1.0) is negative or is greater than or equal to the lower limit for forced convection, C4060(2) (default value 10.0)—no mixed convection regime is considered. Instead, convection heat transfer to the atmosphere is assumed to be given



by the greater of the values defined by the natural and forced convection correlations. This simple and often-used treatment may be specified in MELCOR by deliberate modification of the sensitivity coefficients.

Laminar or turbulent natural convection heat transfer to the atmosphere is determined at a surface by the following criteria:

Region	Criteria	Equation
Laminar Natural Convection	$Ra < 10^9$	(2.85)
Turbulent Natural Convection	$Ra > 10^{10}$	(2.86)
Transition between Laminar and Turbulent Natural Convection	$10^9 \leq Ra \leq 10^{10}$	(2.87)

The constants in Equations (2.85) through (2.87) are implemented as sensitivity coefficient arrays C4061 – C4063 for rectangular, cylindrical, and spherical (hemispherical) geometries.

Laminar or turbulent forced convection heat transfer to the atmosphere is determined at a surface by the following criteria:

Region	Criteria	Equation
Laminar Forced Convection	$Re < 3 \times 10^5$ (rectangular)	(2.88a)
	$Re < 2 \times 10^3$ (cylindrical/spherical)	(2.88b)
Turbulent Forced Convection	$Re > 6 \times 10^5$ (rectangular)	(2.89a)
	$Re > 1 \times 10^4$ (cylindrical/spherical)	(2.89b)
Transition between Laminar and Turbulent Forced Convection	$3 \times 10^5 \leq Re \leq 6 \times 10^5$ (rectangular)	(2.90a)
	$2 \times 10^3 \leq Re \leq 1 \times 10^4$ (cylindrical/spherical)	(2.90b)

The constants in Equations (2.88) through (2.90) are implemented as sensitivity coefficient arrays C4064 – C4066 for rectangular, cylindrical, and spherical (hemispherical) geometries.

The Nusselt number in the transition region is a linear interpolation between the Nusselt numbers for the laminar and turbulent regimes. The interpolation is based on the Rayleigh number for natural convection and the Reynolds number for forced convection. An example is the Nusselt number in the transition region for forced convection with rectangular geometries:

$$Nu_{transition} = \left[ (Re - 3 \times 10^5) / 3 \times 10^5 \right] [Nu_{turbulent} - Nu_{laminar}] + Nu_{laminar} \quad (2.91)$$

The constants in Equation (2.91) are, of course, derived from the sensitivity coefficients that define the limits of laminar and turbulent convection. If the values of these coefficients do not define a proper transition—specifically, if the upper limit for laminar convection, C406m(1) is negative or is greater than or equal to the lower limit for turbulent convection, C406m(2)—no transition regime is considered. Instead, convection heat transfer to the atmosphere is assumed to be given by the greater of the values defined by the laminar and turbulent convection correlations. This simple and often-used treatment may be specified in MELCOR by deliberate modification of the sensitivity coefficients.

#### 2.6.1.1 Conduction/Convection through Liquid Films (film tracking inactive)

Liquid film modeling is discussed in detail in Section 2.8. Heat transfer through a liquid film is accounted for by a heat transfer coefficient,  $H_f$ , which is used in Equations (2.59) and (2.60a). The value of  $H_f$  used when the structure is included in a user-defined film tracking network is discussed in Section 2.6.1.2. When film tracking is inactive, the value of  $H_f$  used is the greater of two values:

- (1) a value obtained from a steady-state correlation appropriate for the geometry and film conditions (zero is used if no film exists) and
- (2) the quotient of the thermal conductivity of the liquid and the transient film thickness. Thus, the liquid film heat transfer coefficient is given by

$$H_f = \max(H_{f,corr}, k_f / \delta_f) \quad (2.92)$$

where

$k_f$  = thermal conductivity of liquid film, W/m•K

$\delta_f$  = liquid film thickness, m

and  $H_{f,corr}$  is a function of surface geometry and film flow conditions. Laminar or turbulent heat transfer through the condensate film is determined by the following criteria:

Laminar if  $Re_f < Re_{LOW,m}$

Turbulent if  $Re_f > Re_{HIGH,m}$

Transition if  $Re_{LOW,m} \leq Re_f \leq Re_{HIGH,m}$

where

$Re_f$  = Reynolds number for the film flow

The laminar heat transfer coefficient through the film,  $h_{f,l}$ , is given by

$$h_{f,l} = (k_f / L) Nu_{f,l}$$

where the laminar film Nusselt number,  $Nu_{f,l}$ , is given by

$$Nu_{f,l} = C_{l,m} \left\{ g \rho_f (\rho_f - \rho_v) h_{fg} L^3 \sin(\theta) / [\mu_f k_f (T_{sat} - T_{srf})] \right\}^{el,m}$$

The turbulent heat transfer coefficient through the film,  $h_{f,t}$ , is given by

$$h_{f,t} = \left\{ k_f / [(\mu_f / \rho_f)^2 / g] \right\}^{et1,m} Nu_{f,t}$$

where the turbulent film Nusselt number,  $Nu_{f,t}$  is given by

$$Nu_{f,t} = (Re_f^{et2,m} + C_{t,m} Re_f^{et3,m} Pr_f^{et4,m})^{et5,m}$$

The transition heat transfer coefficient through the film,  $h_{f,tr}$ , is given by linear interpolation of  $Re_f$  as

$$h_{f,tr} = h'_{f,l} + [h'_{f,t} - h'_{f,l}] \cdot [Re_f - Re_{LOW,m}] / [Re_{HIGH,m} - Re_{LOW,m}]$$

In each of these equations,

$k_f$  = thermal conductivity of film

$L$  = characteristic length of surface

$\rho_f$  = density of film

$\rho_v$  = density of vapor

$g$  = acceleration of gravity

$h_{fg}$  = latent heat of vaporization corrected for sensible heat

$$[h_{fg} + 0.68 c_{p,f} (T_f - T_{srf})]$$

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$c_{p,f}$	= specific heat capacity of film
$T_f$	= temperature of film/atmosphere interface
$T_{srf}$	= temperature of film/structure interface
$\mu_f$	= viscosity of film
$\theta$	= angle between horizontal and structure surface or axis (cyl.)
$h'_{f,l}$	= $h_{f,l}$ evaluated with $Re_f = C42m0(1)$
$h'_{f,t}$	= $h_{f,t}$ evaluated with $Re_f = C42m0(2)$

and

$m$	= 1 for upward-facing rectangular geometries
	= 2 for horizontal cylindrical geometries
	= 3 for spherical or hemispherical geometries

$Re_{LOW,m}$ ,  $Re_{HIGH,m}$  and the minimum permissible value of  $\sin(\theta)$  ( $\cos(\theta)$  for cylindrical geometry) have been implemented as sensitivity coefficients 42m0.  $C_{l,m}$  and  $e_{l,m}$  have been implemented as sensitivity coefficients 42m1, and  $C_{t,m}$  and  $e_{t,m}$  have been implemented as sensitivity coefficients 42m2.

For downward-facing rectangular geometries, the laminar/turbulent transition criteria are given by:

Laminar if  $Ra_f < Ra_{TRAN}$   
 Turbulent, otherwise

where

$Ra_f$  = Rayleigh number for the film flow

The heat transfer coefficient through the film is given by

$$h_f = \left( k_f / \left\{ \sigma_f / [g(\rho_f - \rho_v) \cos(\theta)] \right\}^{1/2} \right) Nu_f$$

where the film Nusselt number is given by

$$Nu_f = C_{l,4} [\max(Ra_{MIN}, Ra_f)]^{el,4}$$

for laminar flow, and by

$$Nu_f = C_{t,4} [\min(Ra_{MAX}, Ra_f)]^{et,4}$$

for turbulent film flow.  $Ra_{TRAN}$ ,  $Ra_{MIN}$ ,  $Ra_{MAX}$  and the minimum value of  $\cos(\theta)$  have been implemented as sensitivity coefficients 4213,  $C_{l,4}$  and  $el,4$  have been implemented as sensitivity coefficients 4214 and  $C_{t,4}$  and  $et,4$  have been implemented as sensitivity coefficients 4215.

Early in its formation, the transient film thickness determines the rate of heat transfer; while its steady-state value is limited by the greater of the correlation value or  $k_f / \delta_{max}$  where  $\delta_{max}$  is the user-specified maximum film thickness discussed in Section 2.8.1 below. Note, that because the film convective heat transfer correlations are functions of the flow conditions, and the flow conditions are a function of the rate of heat transfer, the convective heat transfer coefficient through the film must be determined iteratively as part of the overall solution for the temperature profile through a heat structure and its associated films. This is implied by use of the new time superscript  $(m+1)$ , e.g.,  $H_{f,L}^{m+1}$ .

### 2.6.1.2 Conduction/Convection through Liquid Films (Film Tracking Active)

Section 2.8.2 discusses the film tracking model. This section only describes the correlations used to evaluate heat transfer through films being treated by the film tracking model. The correlations used are the same for all geometries and treat both laminar and turbulent film flow conditions. Laminar or turbulent heat transfer through the condensate film is determined by the following criteria:

Laminar if  $Re_f < Re_{LOW}$   
 Turbulent if  $Re_f > Re_{HIGH}$   
 Transition if  $Re_{LOW} \leq Re_f \leq Re_{HIGH}$

where

$Re_f$  = Reynolds number for the film flow

The laminar heat transfer coefficient through the film,  $h_{f,l}$ , is given by

$$h_{f,l} = k_f / \max(\delta_{f,l}, \delta_{min})$$

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where the laminar film thickness,  $\delta_{f,l}$ , is obtained from the film tracking model solution, and  $\delta_{\min}$  is the user-adjustable minimum film thickness implemented as sensitivity coefficient 4251(1) (see Section 2.8.1). The turbulent heat transfer coefficient through the film,  $h_{f,t}$ , is given by

$$h_{f,t} = \left\{ k_f / \left[ (\mu_f / \rho_f)^2 / (g \cdot \sin(\theta)) \right]^{1/3} \right\} Nu_{f,t}$$

where the turbulent film Nusselt number,  $Nu_{f,t}$ , is given by

$$Nu_{f,t} = \left( Re_f^{et1} + C_t Re_f^{et2} Pr_f^{et3} \right)^{et4}$$

The transition heat transfer coefficient through the film,  $h_{f,tr}$ , is given by linear interpolation of  $Re_f$  as

$$h_{f,tr} = h'_{f,l} + [h'_{f,t} - h'_{f,l}] \cdot [Re_f - Re_{LOW}] / [Re_{HIGH} - Re_{LOW}]$$

In each of these equations,

$k_f$  = thermal conductivity of film

$\rho_f$  = density of film

$g$  = acceleration of gravity

$\mu_f$  = viscosity of film

$\theta$  = angle between horizontal and structure surface or axis (cyl.)

$h'_{f,l}$  =  $h_{f,l}$  evaluated with  $Re_f = C4253(5)$

$h'_{f,t}$  =  $h_{f,t}$  evaluated with  $Re_f = C4253(6)$

$Re_{LOW}$ ,  $Re_{HIGH}$ ,  $C_t$ ,  $et1$ ,  $et2$ ,  $et3$ , and  $et4$  have been implemented as sensitivity coefficients 4253.

## 2.6.2 Radiation Heat Transfer

Simple models are available to determine the energy exchanges between a heat structure surface and the surrounding atmosphere and between the surfaces of heat structures. These are discussed below.

### 2.6.2.1 Atmosphere Radiation Heat Transfer

In addition to the convective boundary condition options, radiative heat transfer between the surface and the boundary volume atmosphere can be specified. Two options are currently available. They are:

- (1) Equivalent band model, and
- (2) Gray gas.

The equivalent band model is based on work by Edwards et al. [3] [4] in which the total radiation properties can be used to adequately calculate radiation heat transfer without resorting to a band model. The equivalent band equation is:

$$q_{EB} = \begin{cases} \sigma(F_g T_g^4 - F_{gw} T_w^4) & \text{for } T_g \neq T_w \\ 0 & \text{for } T_g = T_w \end{cases} \quad (2.93)$$

where

$\sigma$  = Stefan-Boltzmann constant

$F_g = \varepsilon_w \varepsilon_{g1} / (1 - \rho_w \tau_{gb})$

$F_{gw} = \varepsilon_w \alpha_{gw1} / (1 - \rho_w \tau_{gbw})$

$\tau_{gb} = (\varepsilon_{g2} - \varepsilon_{g1}) / \varepsilon_{g1}$

$\tau_{gbw} = (\alpha_{gw2} - \alpha_{gw1}) / \alpha_{gw1}$

and  $\varepsilon$  and  $\alpha$  are the emissivity and absorptivity, respectively. Subscripts  $g$ ,  $w$ ,  $gw$ , 1, and 2 refer to the gas, the wall, the gas at the wall temperature, one path length, and two path lengths. The values of the gas emissivity ( $\varepsilon_g$ ) and absorptivity ( $\alpha_{gw}$ ), obtained from the model in CONTAIN [5], are functions of the gas composition, including the pressure of water vapor, CO, and CO<sub>2</sub> as well as the radiation path length, which is user specified. The wall emissivity  $\varepsilon_w$ , is given by user input,  $\varepsilon_{w,user}$ , that is overwritten if a liquid film is present. The emissivity of the film-covered wall becomes

$$\varepsilon_w = 1 - \rho_f - \rho_w \tau_f / (1 - \rho_f \rho_w) \quad (2.94a)$$

where

$$\tau_f = \exp(-1000\delta) \quad (2.94b)$$

$$\rho_f = (1 - \varepsilon_{H_2O})(1 - \tau_f) \quad (2.94c)$$

$$\rho_w = 1 - \varepsilon_{w,user} \quad (2.94d)$$

$$\varepsilon_{H_2O} = 0.96$$

and  $\delta$  is the film thickness in meters.

The gray gas model equation is:

$$q_{GG} = \sigma \left[ (1/\varepsilon_g) + (1/\varepsilon_w) - 1 \right]^{-1} (T_g^4 - T_w^4) \quad (2.95)$$

where the gas emissivity is calculated for one path length.

### 2.6.2.2 Structure-to-Structure Radiation Heat Transfer

Structure-to-structure radiation can be calculated by a simple gray surface model. This optional model assumes that the radiative exchange between pairs of surfaces is independent and decoupled from the exchanges involved with other surfaces or with the intervening atmosphere. This permits sequential processing for each pair and does not require the use of iterative or simultaneous solution techniques. The net radiative heat loads for the surfaces of each heat structure are entered explicitly into the surface nodal energy balances similar to the method described in Section 2.3.2 for surface power sources.

An arbitrary number of heat structure surface pairs may be defined by the user and radiative exchange calculated between the surfaces of each pair by the following relationship:

$$q_{12} = \frac{\sigma(T_1^4 - T_2^4)}{\frac{1 - \varepsilon_1}{\varepsilon_1 A_1} + \frac{1}{A_1 F_{12}} + \frac{1 - \varepsilon_2}{\varepsilon_2 A_2}} \quad (2.96)$$



where

$q_{12}$	= radiative energy transfer rate from surface 1 to surface 2 (W)
$\sigma$	= Stefan-Boltzmann constant ( $\text{W/m}^2 \cdot \text{K}^4$ )
$T_1$	= surface 1 temperature (K)
$T_2$	= surface 2 temperature (K)
$\varepsilon_1$	= surface 1 emissivity
$\varepsilon_2$	= surface 2 emissivity
$A_1$	= surface 1 area ( $\text{m}^2$ )
$A_2$	= surface 2 area ( $\text{m}^2$ )
$F_{12}$	= view factor from surface 1 to surface 2

The emissivities may be computed by a default relation (from the COR package for oxidized steel surfaces) or may be computed by evaluation of user-specified real-valued control functions. A modification to account for the presence of a water film on either surface is applied and is the same as that described in Section 2.6.2.1 for radiative exchanges with the atmosphere. The areas used in the above equation correspond to the uncovered portions above the swollen liquid level of the adjacent CVH control volume. Radiative energy exchange between the surfaces of a pair is not calculated (i.e.,  $q_{12}$  is set to 0.0) when:

- (1) either of the surfaces is covered by a pool,
- (2) either of the surface emissivities is determined to be zero, or
- (3) the input view factor is zero.

### 2.6.3 Pool Convection Heat Transfer

Natural, forced, or mixed convection heat transfer to the pool is determined at a surface by the following criteria:

Region	Criteria	Equation
Natural Convection	$\text{Re}^2 < 1.0Gr$	(2.97)
Forced Convection	$\text{Re}^2 > 10.0Gr$	(2.98)

Mixed Convection	$1.0Gr \leq Re^2 \leq 10.0Gr$	(2.99)
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where

$Re$  = Reynolds number for pool

$Gr$  = Grashof number for pool

$Ra$  = Rayleigh number for pool

The constants in Equations (2.97) through (2.99) are implemented as sensitivity coefficient array C4080.

The pool natural convection heat transfer correlations have the following form:

$$Nu = C Ra^m + D \quad (2.100)$$

where

$Nu$  = Nusselt number

$Ra$  = Rayleigh number

$C, m, D$  = constants dependent on flow condition and geometry

The constants  $C$ ,  $m$ , and  $D$  in Equation (2.100) have been implemented as sensitivity coefficient arrays C4151 – C4162 and default values are presented in Table 2.3 for the various flow conditions and geometries.

The pool forced convection heat transfer correlations have the following form:

$$Nu = C Re^m Pr^n + D \quad (2.101)$$

where

$Nu$  = Nusselt number

$Re$  = Reynolds number

$Pr$  = Prandtl number

$C, m, n, D$  = constants dependent on flow condition and geometry

The constants  $C$ ,  $m$ ,  $n$ , and  $D$  in Equation (2.101) have been implemented as sensitivity coefficient arrays C4163 – C4174 and are presented in Table 2.3 for the various flow conditions and geometries.

The Nusselt number in the mixed convection regime is a linear interpolation between the Nusselt numbers for the natural and forced convection regimes, based on the ratio  $Re^2/Gr$ . This is the same method employed for atmosphere heat transfer, and an example is shown in Section 2.6.1. As with atmosphere heat transfer, the sensitivity coefficients defining the limits of natural and forced convection (sensitivity coefficient array C4080) may be chosen to eliminate the mixed convection regime for the pool in favor of use of the maximum of natural and forced convection heat transfer.

Laminar or turbulent natural convection heat transfer to the pool is determined at a surface by the following criteria:

Region	Criteria	Equation
Laminar Natural Convection	$Ra < 10^9$	(2.102)
Turbulent Natural Convection	$Ra > 10^{10}$	(2.103)
Transition between Laminar and Turbulent Natural Convection	$10^9 \leq Ra \leq 10^{10}$	(2.104)

The constants in Equations (2.102) through (2.104) are implemented as sensitivity coefficient arrays C4081 – C4083 for rectangular, cylindrical, and spherical (hemispherical) geometries.

Laminar or turbulent forced convection heat transfer to the pool is determined at a surface by the following criteria:

Region	Criteria	Equation
Laminar Forced Convection	$Re < 3 \times 10^5$ (rectangular)	(2.105a)
	$Re < 2 \times 10^3$ (cylindrical/spherical)	(2.105b)
Turbulent Forced Convection	$Re > 6 \times 10^5$ (rectangular)	(2.106a)
	$Re > 1 \times 10^4$ (cylindrical/spherical)	(2.106b)
Transition between Laminar and Turbulent Forced Convection	$3 \times 10^5 \leq Re \leq 6 \times 10^5$ (rectangular)	(2.107a)
	$2 \times 10^3 \leq Re \leq 1 \times 10^4$ (cylindrical/spherical)	(2.107b)

The constants in Equations (2.105) through (2.107) are implemented as sensitivity coefficient arrays C4084 – C4086 for rectangular, cylindrical, and spherical (hemispherical) geometries.

The Nusselt number in the transition region is a linear interpolation between the Nusselt numbers for the laminar and turbulent regimes. The interpolation is based on the Rayleigh number for natural convection and the Reynolds number for forced convection. This is the same method employed for atmosphere heat transfer, and an example is shown in Section 2.6.1. As with atmosphere heat transfer, the sensitivity coefficients defining the limits of laminar and turbulent convection (sensitivity coefficient arrays C408m) may be chosen to eliminate the transition regime for the pool in favor of use of the maximum of laminar and turbulent convection heat transfer.

#### 2.6.4 Pool Boiling Heat Transfer

If a heat structure is submerged in a pool or a film is present and the heat structure surface temperature,  $T_{surf}$ , is greater than the saturation temperature,  $T_{sat}$ , at the total control volume pressure, pool boiling heat transfer from the heat structure is assumed. Using the heat structure surface temperature and various liquid properties, the logic for choosing the appropriate pool boiling regime is given by:

Nucleate boiling (Rohsenow) is calculated if

$$q''_{nb} \text{ (Rohsenow)} \leq q''_{chf} \text{ (Zuber)}$$

Film boiling (modified Bromley) is calculated if

$$q''_{film} \text{ (modified Bromley)} \geq q''_{mfilm} \text{ (Zuber)}$$

where

$$q''_{nb} = \text{nucleate boiling heat flux given by Equation (2.108), W/m}^2$$

$$q''_{chf} = \text{critical heat flux given by Equation (2.110), W/m}^2$$

$$q''_{film} = \text{film boiling heat flux given by Equation (2.112), W/m}^2$$

$$q''_{mfilm} = \text{minimum film boiling heat flux given by Equation (2.111), W/m}^2$$

If neither of these conditions is met, the surface is in transition boiling and a linear interpolation of the surface temperature is used to determine the heat flux at that temperature.

For all the above cases, once a heat flux has been determined, an effective heat transfer coefficient is evaluated as the ratio of heat flux over the difference between the surface

and pool temperatures. This heat transfer coefficient is used as the boundary heat transfer coefficient in the solution of the heat conduction equations.

### 2.6.4.1 Nucleate Boiling

The nucleate boiling heat flux is obtained through the Rohsenow relation [6]

$$\left[ \frac{c_{pl}(T_{surf} - T_{sat})}{h_{fg}} \right] = C_{sf} \left[ \frac{q''_{nb}}{\mu h_{fg}} \left( \frac{\sigma}{g(\rho_l - \rho_v)} \right)^{1/2} \right]^n Pr^m \quad (2.108)$$

where

$q''_{nb}$	= nucleate boiling heat flux, W/m <sup>2</sup>
$c_{pl}$	= heat capacity of liquid at $T_{sat}$ , J/kg•K
$T_{surf}$	= temperature of surface, K
$T_{sat}$	= saturation temperature in boundary volume, K
$C_{sf}$	= constant determined empirically for different surfaces and fluids (default = 0.013)
$\mu$	= dynamic viscosity of liquid at $T_{avg}$ , kg/m•s
$h_{fg}$	= latent heat in boundary volume of this surface, J/kg
$\sigma$	= surface tension at $T_{avg}$ , N/m
$g$	= acceleration of gravity, m/s <sup>2</sup>
$\rho_l$	= density of liquid at $T_{sat}$ , kg/m <sup>3</sup>
$\rho_v$	= density of vapor at $T_{sat}$ , kg/m <sup>3</sup>
$n$	= constant (default = 0.33)
Pr	= Prandtl number of liquid in boundary volume
$m$	= constant (default = 1.0)
$T_{avg}$	= $(T_{surf} + T_{sat}) / 2$ , K

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The constants  $C_{sf}$ ,  $m$ , and  $n$  in Equation (2.108) have been implemented as sensitivity coefficient array C4180.

The surface tension of water is given as a function of temperature by

$$\sigma = 0.2358(1 - 0.625 T_R) T_R^{1.256} + c \quad (2.109)$$

where

- $\sigma$  = surface tension, N/m
- $T$  = temperature, K
- $T_R$  =  $1 - T / 647.3$
- $c$  = constant (default = 0.0)

The constants in Equation (2.109), including  $c$ , have been implemented as sensitivity coefficient array C4000.

### 2.6.4.2 Critical Heat Flux

The critical heat flux is given by

$$q''_{CHF} = 0.18 \rho_v h_{fg} [\sigma (\rho_l - \rho_v) g / \rho_v^2]^{1/4} [\rho_l / (\rho_l + \rho_v)]^{1/2} \quad (2.110)$$

where

- $q''_c$  = critical heat flux, W/m<sup>2</sup>
- $\rho_v$  = density of vapor at  $T_{sat}$ , kg/m<sup>3</sup>
- $\rho_l$  = density of liquid at  $T_{sat}$ , kg/m<sup>3</sup>
- $h_{fg}$  = latent heat in boundary volume, J/kg
- $g$  = acceleration of gravity, m/s<sup>2</sup>
- $\sigma$  = surface tension at  $T_{avg}$ , N/m
- $T_{avg}$  =  $(T_{surf} + T_{sat}) / 2$ , K

$T_{sat}$  = saturation temperature in boundary volume, K

$T_{surf}$  = temperature of this surface, K

The constants in Equation (2.110) have been implemented as sensitivity coefficient array C4181. Zuber gives a leading coefficient of 0.131, while 0.18 is the value suggested by Rohsenow, see Reference [5].

#### 2.6.4.3 Minimum Film Boiling Heat Flux

The minimum film boiling heat flux is given by Zuber [5] as

$$q''_{mfilm} = 0.09 \rho_v h_{fg} [\sigma(\rho_l - \rho_v)g/\rho_l^2]^{1/4} [\rho_l/(\rho_l + \rho_v)]^{1/2} \quad (2.111)$$

where

$q''_{mfilm}$  = minimum film boiling heat flux, W/m<sup>2</sup>

The constants in Equation (2.111) have been implemented as sensitivity coefficient array C4182.

#### 2.6.4.4 Stable Film Boiling

The film boiling heat flux is given by Bromley [5] as

$$q''_{film} = 0.943 [\rho_v(\rho_l - \rho_v)g k_v^3 (h_{fg} + (1/2)c_{pv}\Delta T)/\mu_v L_c]^{1/4} \Delta T^{0.75} \quad (2.112)$$

where

$q''_{film}$  = film boiling heat flux, W/m<sup>2</sup>

$L_c$  = characteristic length of this surface, m

$\Delta T$  =  $T_{surf} - T_{sat}$ , K

$T_{surf}$  = temperature of this surface, K

$T_{sat}$  = saturation temperature in boundary volume, K

$g$  = acceleration due to gravity, m/s<sup>2</sup>

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$h_{fg}$	= latent heat in boundary volume, J/kg
$\rho_l$	= density of liquid at $T_{sat}$ , kg/m <sup>3</sup>
$\rho_v$	= density of vapor at $T_{sat}$ , kg/m <sup>3</sup>
$c_{pv}$	= heat capacity of vapor at $T_{sat}$ , J/kg•K
$T_{avg}$	= $(T_{surf} + T_{sat}) / 2$ , K
$\mu_v$	= dynamic viscosity of vapor at $T_{avg}$ , kg/m•s
$k_v$	= thermal conductivity of vapor at $T_{avg}$ , W/m•K

The constants in Equation (2.112) have been implemented as sensitivity coefficient array C4183.

### 2.6.4.5 Transition Boiling

If transition boiling occurs at a surface, the heat flux is calculated as follows. First the surface temperatures at critical heat flux and minimum film boiling are calculated from

$$T_c = T_{sat} + (q_c'' \Delta T^3 / q_{NB}'')^{1/3} \quad (2.113)$$

$$T_{mfilm} = T_{sat} + [q_{mfilm}'' \Delta T^{0.75} / (q_{film}'' + q_{rad}'')]^{4/3} \quad (2.114)$$

where

$T_{sat}$	= saturation temperature in boundary volume, K
$\Delta T$	= $T_{surf} - T_{sat}$ , K
$q_c''$	= critical heat flux given by Equation (2.110), W/m <sup>2</sup>
$q_{NB}''$	= nucleate boiling heat flux given by Equation (2.108), W/m <sup>2</sup>
$q_{mfilm}''$	= minimum film boiling heat flux given by Equation (2.111), W/m <sup>2</sup>
$q_{film}''$	= film boiling heat flux given by Equation (2.112), W/m <sup>2</sup>
$q_{rad}''$	= radiation to pool heat flux given by Equation (2.116), W/m <sup>2</sup>



The constants in Equations (2.113) and (2.114) are sensitivity coefficients 4180(4) and 4183(3), respectively.

With these temperatures known, the transition boiling heat flux is then obtained by logarithmic interpolation between the critical heat flux and the minimum film boiling heat flux based on  $(T - T_{sat})$  values and includes the radiation heat flux. Therefore, after simplification, the transition boiling heat flux is given by

$$q''_{tran} = \exp\left(\frac{\ln(q''_c)(\ln \Delta T_{surf} - \ln \Delta T_{mfilm}) + \ln(q''_{mfilm})(\ln \Delta T_c - \ln \Delta T_{surf})}{\ln \Delta T_c - \ln \Delta T_{mfilm}}\right) + q''_{rad} \quad (2.115)$$

where

$$q''_{tran} = \text{transition boiling heat flux, W/m}^2$$

$$T_c = \text{critical temperature, K}$$

$$\Delta T_{surf} = T_{surf} - T_{sat}, \text{ K}$$

$$\Delta T_{mfilm} = T_{mfilm} - T_{sat}, \text{ K}$$

$$\Delta T_c = T_c - T_{sat}, \text{ K}$$

$$q''_{rad} = \text{radiation heat flux calculated by Equation (2.116), W/m}^2$$

#### 2.6.4.6 Radiation During Boiling

Radiation heat transfer between a surface and the boundary volume pool is calculated during stable film and transition boiling. The radiation to pool heat flux is given by

$$q''_{rad} = C \sigma (T_{surf}^4 - T_{pool}^4) \quad (2.116)$$

where

$$q''_{rad} = \text{radiation to pool heat flux, W/m}^2$$

$$T_{surf} = \text{temperature of surface, K}$$

$$T_{pool} = \text{temperature of pool in boundary volume, K}$$

$$\sigma = \text{Stefan-Boltzmann constant, } 5.669 \times 10^{-8} \text{ W/m}^2 \cdot \text{K}^4$$

The constant C in Equation (2.116) defaults to 1.0 and has been implemented as sensitivity coefficient array C4184.

## 2.6.5 Energy Transfer to Control Volumes

The energy that is transferred from a heat structure surface to the boundary volume pool is:

$$\Delta Q_{pool}^m = q_{pool}''^m x_{pool} A \Delta t_m \quad (2.117)$$

Likewise, the energy that is transferred from a heat structure surface to the boundary volume atmosphere is:

$$\Delta Q_{atm}^m = q_{atm}''^m (1 - x_{pool}) A \Delta t_m \quad (2.118)$$

where

$\Delta Q_{pool}^m$  = energy transferred between heat structure surface and pool between times  $t_{m-1}$  and  $t_m$ , J

$\Delta Q_{atm}^m$  = energy transferred between heat structure surface and atmosphere between times  $t_{m-1}$  and  $t_m$ , J

$q_{pool}''^m$  = heat flux to pool at time  $t_m$ , W/m<sup>2</sup>

$q_{atm}''^m$  = heat flux to atmosphere at time  $t_m$ , W/m<sup>2</sup>

$A$  = heat structure boundary surface area, m<sup>2</sup>

$x_{pool}$  = fraction of boundary surface in pool of boundary volume

$\Delta t_m$  = timestep size ( $t_m - t_{m-1}$ ), s

These time-surface integrals are evaluated at each boundary surface to determine the total energy transferred between each heat structure and its respective boundary volume atmosphere and pool. These integrals are used to update the energy communication arrays for the CVH package.

## 2.7 Mass Transfer

Condensation occurs on a structure surface if its temperature is below the dew point of the associated atmosphere, and mass transfer from that surface has been enabled through user input (see the description for record HSCCCCC400 in the HS Users' Guide). The dew point is the saturation temperature corresponding to the partial pressure of steam in the bulk atmosphere of the boundary volume (obtained from the CVH data base). Evaporation from an existing film on a heat structure surface occurs if the surface temperature of the film exceeds the dew point. (A model to treat film flashing at the structure/film interface, when the temperature exceeds the boiling temperature, has not been activated because it has been unnecessary.)

In nearly pure steam environments, the rate of condensation is limited only by heat transfer through the structure, i.e. by the ability of the structure to dissipate the latent heat of vaporization that is released by condensation. Hence, in nearly pure steam environments, the rates of condensation and evaporation will self-adjust to whatever values are required to maintain the saturation temperature at the film/atmosphere interface.

As noncondensibles are introduced into the condensing steam, their accumulation near the film surface from local steam depletion tends to inhibit the flow of fresh steam to the film surface and restricts the rate of condensation. Consequently, when the ratio of the steam partial pressure to the total pressure in the boundary volume (obtained from the CVH data base) falls below a user-prescribed threshold, VPFRAC (also sensitivity coefficient 4200 with a default value of 0.9995), a mass transfer rate limitation is imposed on the rate of condensation. Experimental evidence indicates that the value of VPFRAC (below which diffusion rate limitations to condensation mass transfer become significant) can depend on the degree of turbulence. As the turbulence decreases, the value of VPFRAC should be increased to account for the inhibiting effect of even very small amounts of noncondensibles in a stagnant environment. Conversely, in a well-mixed system, the value of VPFRAC may have to be reduced to avoid artificially limiting the condensation rate. It is suggested that the user vary the value of VPFRAC in sensitivity studies, if uncertainty in the rate of condensation is of much concern.

The mass transfer rate limitation is a function of the diffusion mass transfer coefficient, which is calculated at a heat structure boundary surface whenever the surface is exposed to the atmosphere of its boundary volume. This coefficient is related to the atmosphere Nusselt number through a heat transfer analogy and is calculated by a Sherwood number correlation involving the Nusselt, Prandtl, and Schmidt numbers. This correlation is presented in Section 2.7.1.

The mass transfer rate-limited expression for condensation or evaporation at a surface exposed to a noncondensable-bearing atmosphere is formulated using a mechanistic approach which models the diffusion of a condensable vapor through a gas layer that contains noncondensable gases. Section 2.7.2 discusses this expression. If the surface temperature is greater than the critical temperature, 647.2°K, diffusion mass transfer is

not calculated. However, the diffusion mass transfer coefficient is still calculated using Equation (2.124) since the radionuclide package requires this quantity.

### 2.7.1 Sherwood Number for Diffusion Mass Transfer

The mass transfer coefficient is related to the atmosphere Nusselt number by a heat and mass transfer analogy. In addition to the use of the Nusselt, Reynolds, and Prandtl numbers, the HS package uses the following dimensionless variables for its mass transfer calculations:

$$\text{Schmidt number } (Sc) = \mu / (\rho D)$$

$$\text{Sherwood number } (Sh) = h_D L_c / D$$

where

$\mu$  = dynamic viscosity of atmosphere at average of surface and atmosphere temperatures, kg/m•s

$\rho$  = density of atmosphere, kg/m<sup>3</sup>

$D$  = diffusivity, m<sup>2</sup>/s

$h_D$  = mass transfer coefficient, m/s

$L_c$  = characteristic length or dimension of surface, m

A Sherwood number correlation is used to calculate a diffusion mass transfer coefficient. The correlation is

$$Sh = C Nu^a Sc^b Pr^d \quad (2.119)$$

where

$Nu$  = Nusselt number

$Pr$  = Prandtl number

The constants  $C$ ,  $a$ ,  $b$ , and  $d$  have been implemented as sensitivity coefficient array C4201. The default values are:

$C$  = 1.0

$$a = 1.0$$

$$b = 1/3$$

$$d = -1/3$$

The mass transfer coefficient is then obtained by

$$h_D = F_m Sh D / L_c \quad (2.120)$$

where  $F_m$  is an arbitrary, nonnegative scaling factor (with a default value of 1.0) that may be specified by the user at any surface. Refer to Section 2.6 for further discussion of this scaling factor and a caution concerning its use.

## 2.7.2 Condensation and Evaporation with Noncondensibles

The principal expression for condensation or evaporation mass flux at a surface exposed to an atmosphere with a significant partial pressure of noncondensable gases (i.e.,  $P_{stm} < VPFRAC \times P_{tot}$ ) is formulated using a mechanistic approach which models the diffusion of a condensable vapor through a gas layer that contains noncondensable gases [5]. The condensation mass flux is given by:

$$\dot{m}_c = h_D \rho_v \ln(\Delta P_{srf} / \Delta P_{atm}) \quad (2.121)$$

where

$$\dot{m}_c = \text{mass flux at this surface, kg/m}^2 \cdot \text{s}$$

$$h_D = \text{mass transfer coefficient, m/s}$$

$$\rho_v = \text{density of vapor at } T_{sat}(P_{tot}), \text{ kg/m}^3$$

$$\Delta P_{srf} = P_{tot} - P_{srf}, \text{ Pa}$$

$$\Delta P_{atm} = P_{tot} - P_{stm}, \text{ Pa}$$

$$P_{tot} = \text{total control volume pressure, Pa}$$

$$P_{srf} = \text{saturation pressure of steam at the surface temperature, Pa}$$

$$P_{stm} = \text{steam partial pressure in the control volume, Pa}$$

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Because Equation (2.121) is singular when the  $P_{srf}$  reaches  $P_{tot}$  it is necessary to bound the rate of evaporation as the surface temperature reaches  $T_{sat}(P_{tot})$ . This is done by using a flashing heat transfer coefficient to limit the rate of evaporation as follows:

$$\dot{m}_e = h_e \min(0, T_{dew} - T_{srf}) / h_{fg} \quad (2.122)$$

$$\dot{m} = \max(\dot{m}_c, \dot{m}_e) \quad (2.123)$$

where

$h_e$  = flashing heat transfer coefficient,  $W/m^2 \cdot K$

$h_{fg}$  = latent heat of vaporization for steam,  $J/kg$

$T_{dew}$  = control volume dew point temperature,  $K$

$T_{srf}$  = surface temperature,  $K$

and  $h_e$  has been implemented as sensitivity coefficient 4202, with a default value of  $5 \times 10^5 W/m^2 \cdot K$ .

### 2.7.3 Mass-Energy Transfer to Control Volumes

The mass which is transferred between the surface of a heat structure and the atmosphere of its boundary volume between times  $t_{m-1}$  and  $t_m$  is the value of the integral from  $t_{m-1}$  to  $t_m$  of the product of the mass flux and the area of the surface which is exposed to the atmosphere:

$$\Delta m^m = \dot{m} A (1 - x_{pool}) \Delta t_m \quad (2.124)$$

where

$\Delta m^m$  = mass transferred between heat structure surface and atmosphere between times  $t_{m-1}$  and  $t_m$ ,  $kg$

$\dot{m}$  = mass flux at heat structure surface,  $kg/m^2 \cdot s$

$A$  = heat structure boundary surface area,  $m^2$

$x_{pool}$  = fraction of boundary surface in pool of boundary volume

$\Delta t_m$  = system timestep size ( $t_m - t_{m-1}$ ), s

Mass transfer is not considered if the pool fraction is greater than the critical pool fraction CPFAL for the structure as defined in Section 2.4.

The time-surface integral of the mass flux is evaluated during each computational cycle for each surface to determine the total mass of the liquid on each heat structure boundary surface. Its value is constrained so that no more steam is condensed than is present in its boundary volume and no more liquid is evaporated or flashed than is present on the surface.

If more than a user-specified fraction (sensitivity coefficient 4203(2), with a default value of 90%) of the steam in a control volume is condensed during a computational cycle, then remedial action is taken. If the current timestep size is greater than a user-specified value (sensitivity coefficient 4203(1), with a default value of -1. s), then the HS package requests that the computational cycle be repeated with a smaller timestep size to eliminate the excessive condensation. The requested timestep size is equal to the current value times the ratio of the maximum amount of steam that may condense divided by the actual, excessive amount that would have condensed without the requested fallback. If the current timestep size is less than the value prescribed by sensitivity coefficient 4203(1), then the condensation flux (mass transfer rate) on each surface associated with this boundary volume is reduced by the same factor that would have been applied to the timestep size with the fallback option. The HS (not the entire MELCOR cycle) calculation is then repeated with the modified mass transfer rates. The fallback option is the default and recommended option because it does not alter the mechanistically calculated condensation rates. The scaling option may falsify the solution and should be avoided, if possible. Excessive condensation is a result of violating a timestep size constraint imposed by the explicit coupling between the HS and CVH packages (and is akin to the material Courant timestep limit). In some situations, it may be possible to avoid excessive condensation by re-nodalizing the problem to reduce the ratio of the surface area for condensation to the volume of steam available for condensation.

The liquid mass which is transferred to a heat structure surface by other packages is obtained from an array in the HS package data base whose elements are updated using an interface routine that can be called by any package.

For each heat structure surface, the mass and energy transfer is calculated for the steam which was condensed from or added to its boundary volume atmosphere and the liquid deposited in the boundary volume pool. The results of these calculations are used to update the mass and energy communication arrays for the CVH package. If the heat structure surface is part of a film tracking network, then the film thickness will be determined dynamically as a function of the film flow rate and the drainage from the surface will be partitioned between the boundary volume pool, the boundary volume fog

and the surfaces of other heat structures in the user-specified network. The film tracking model is discussed in Section 2.8.2.

## 2.8 Liquid Film Modeling

The mass, thickness, and specific enthalpy of a liquid film on a heat structure boundary surface are first determined during the initialization procedure in MELGEN execution. Calculation of these properties is also carried out during MELCOR execution. The models that are used to determine liquid film properties are described in Section 2.8.1. Section 2.8.2 describes the film tracking model, which is based on the model in CONTAIN [4] and is user-activated to track film drainage over a user-specified network of connected structure surfaces.

### 2.8.1 Film Models

During MELGEN and MELCOR execution, the mass of a liquid film on a heat structure boundary surface is determined from

- (1) calculation of the mass which is transferred between this surface and its boundary volume by condensation, evaporation or draining,
- (2) the liquid mass which is transferred to this surface by other packages, and
- (3) the liquid mass which is transferred to this surface by external sources (tabular function or control function) or film drainage from other heat structure surfaces, if the surface is part of a user-defined film tracking network.

The mass of the liquid film and the film surface and structure surface temperatures enable its thickness and specific enthalpy to be determined. The film equations are nodalized so that half of the film mass is associated with the film/structure interfacial node and the other half is associated with the atmosphere/film interfacial node. Therefore, the average specific enthalpy of the film is given by  $0.5 \cdot [h_f(T_{s,srf}) + h_f(T_{f,srf})]$ , where  $h_f(T)$  is the specific enthalpy of the film at temperature  $T$ ,  $T_{s,srf}$  is the film/structure interfacial temperature and  $T_{f,srf}$  is the atmosphere/film interfacial temperature.

For structures which are not part of a film tracking network, the condensate and deposited liquid is permitted to accumulate on a surface until the film thickness reaches a maximum. If the liquid mass is sufficiently large that the film thickness exceeds this maximum, then the excess liquid is deposited in the pool of the boundary volume of the surface. The maximum thickness of a liquid film on a surface is determined in one of two ways:

- (1) for geometries for which the convective heat transfer coefficient through the film (see Section 2.6.1.1) is obtained from a correlation as a function of the Reynolds number of the film flow, the Reynolds number is also used to obtain the film



thickness from the correlations used by the film tracking model (see Section 2.8.2 below) or

- (2) for all other geometries the maximum film thickness is obtained from a user-adjustable value. The user-adjustable value,  $\delta_{\max}$ , has been implemented as sensitivity coefficient 4251(2) with a default value of  $5 \times 10^{-4}$  m.

## 2.8.2 Film Tracking Model

For structures which are part of a film tracking network, the film thickness on a surface is determined iteratively as a function of the Reynolds number of the film flow rate as follows. First, the Reynolds number of the film flow is given by

$$Re_f = 2(\dot{m}_{in} + \dot{m}_{out}) / (w \mu_f) \quad (2.125)$$

where  $\dot{m}_{in}$  is the mass inflow rate (kg/s) from film drainage to the surface from other surfaces in the network and water deposited on the surface by other MELCOR packages,  $\dot{m}_{out}$  is the mass outflow rate (kg/s) from film drainage from this surface (which is to be determined iteratively),  $w$  is the width of this surface and  $\mu_f$  is the bulk viscosity of the film. As an initial guess  $\dot{m}_{out}$  is set equal to zero. The film thickness as a function of  $Re_f$  is given by the following correlation

$$\begin{aligned} \delta_f &= C_{f,l} \cdot \delta^* \cdot Re_f^{ef,l}, \text{ if } Re_f < Re_{LAM} \\ &= C_{f,t} \cdot \delta^* \cdot Re_f^{ef,t}, \text{ if } Re_f > Re_{TURB} \\ &= \text{determined by interpolation between limits at } Re_{LAM} \text{ and } Re_{TURB}, \text{ otherwise} \end{aligned} \quad (2.126)$$

$$\delta^* = [(\mu_f / \rho_f)^2 / (g \cdot \sin \theta)]^{1/3}$$

where the constants  $C_{f,x}$ , exponents  $ef,x$  and limits  $Re_x$  (where  $x$  represents laminar or turbulent) in Equation (2.126) have been implemented as sensitivity coefficients 4253, and  $\rho_f$  and  $\theta$  are the film density and angle of inclination of the surface from horizontal, respectively. The film thickness can also be determined from the conservation of film mass as

$$\delta_f = [m_{f,0} + (\dot{m}_{in} + \dot{m}_c - \dot{m}_{out}) \cdot \Delta t] / (\rho_f A_{srf}) \quad (2.127)$$

where  $m_{f,0}$  is the film mass at the start of the timestep  $\Delta t$ ,  $\dot{m}_c$  is the condensation rate (a negative value indicates evaporation) and  $A_{srf}$  is the surface area. Equation (2.127) has been presented for the case of rectangular geometry; the equations for cylindrical and spherical geometry are different because the film thickness is related to film volume differently.

For given values of  $m_{f,0}$ ,  $\dot{m}_{in}$ , and  $\dot{m}_c$ , Equations (2.126) and (2.127) can be solved simultaneously by iterating on the value of  $\dot{m}_{out}$  to determine consistent values of  $\delta_f$  and  $\dot{m}_{out}$ . Note, however, that if the value of  $\delta_f$  given by Equation (2.126) with  $\dot{m}_{out} = 0$  exceeds the value of  $\delta_f$  given by Equation (2.127) with  $\dot{m}_{out} = 0$ , then the film thickness cannot possibly achieve the steady-state value consistent with Equation (2.126) during the given timestep. When a steady-state value consistent with Equation (2.126) is impossible for a timestep,  $\dot{m}_{out}$  is set equal to zero and Equation (2.127) is used to determine  $\delta_f$ .

A user-specified minimum film thickness,  $\delta_{min}$ , has been implemented as sensitivity coefficient 4251(1) to prevent film flow when the film thickness is less than the specified value (default value is  $10^{-9}$  m). This can be used to inhibit film flow on rough surfaces until a reasonably thick film is established. Hence, when the solution to Equations (2.126) and (2.127) is less than  $\delta_{min}$ , then  $\delta_f$  in Equation (2.127) is set equal to  $\delta_{min}$  to determine the value of  $\dot{m}_{out}$ , if a positive value is possible; otherwise,  $\delta_f$  is equal to the value obtained from Equation (2.127) with  $\dot{m}_{out}$  set equal to zero.

The outflow (drainage) from the film tracking solution,  $\dot{m}_{out}$ , is partitioned between the CVH pool associated with the surface, "rain" passed to the SPR package via the TP package and the other drainage surfaces associated with the given surface through the user-specified film tracking network.

## 2.9 Stored Energy of a Heat Structure

The total stored energy of each heat structure, including surface films, is initialized during MELGEN execution. The stored energy of the structure itself is obtained by integrating the product of the volumetric heat capacity weight and the absolute temperature over the volume of the heat structure. The energy of the films is added to that total to arrive at a total structure energy storage. Therefore, the initial stored energy is

$$E^0 = f \sum_{i=1}^N G_i^m T_i^0 + m_{film,L}^0 h_{film,L}^0 + m_{film,R}^0 h_{film,R}^0 \quad (2.128)$$

where

$E^0$	= initial stored energy of heat structure, J
$f$	= geometry factor with the following values for different geometries, = surface area of heat structure for rectangular geometries, m <sup>2</sup> = axial length of heat structure for cylindrical geometries, m = 1.0 for spherical and hemispherical geometries.
$G_i^0$	= volumetric heat capacity weight  = $C_{p,i}^0 HVR$ for $i = 1$  = $C_{p,i-1}^0 HVL_i + C_{p,i}^0 HVR_i$ for $i = 2, \dots, N - 1$  = $C_{p,i-1}^0 HVL_i$ for $i = N$
$C_{p,i}^0$	= initial volumetric heat capacity of mesh interval $i$ , J/m <sup>3</sup> •K
$HVL_i$	= left (inside) volume weight for mesh interval $i$ , defined in Sections 2.1.1 and 2.2.1
$HVR_i$	= right (outside) volume weight for mesh interval $i$ , defined in Sections 2.1.1 and 2.2.1
$T_i^0$	= initial temperature of node $i$ , K
$T_{i-1}^0$	= initial temperature of node $i - 1$ , K
$m_{film,L}^0$	= initial mass of film on left boundary surface, kg
$h_{film,L}^0$	= initial specific enthalpy of film on left boundary surface, J/kg
$m_{film,R}^0$	= initial mass of film on right boundary surface, kg
$h_{film,R}^0$	= initial specific enthalpy of film on right boundary surface, J/kg

During MELCOR execution, the change in the stored energy of each heat structure is calculated every cycle. This is obtained by integrating the product of the volumetric heat capacity weight and the change in temperature between times  $t_{m-1}$  and  $t_m$  over the volume of the heat structure, and including the energy change of the surface films. Therefore,

$$\Delta E^m = f \sum_{i=1}^N G_i^m (T_i^m - T_i^{m-1}) + m_{film,L}^m h_{film,L}^m - m_{film,L}^{m-1} h_{film,L}^{m-1} + m_{film,R}^m h_{film,R}^m - m_{film,R}^{m-1} h_{film,R}^{m-1} \quad (2.129)$$

where

$\Delta E^m$  = change in stored energy of heat structure between times  $t_{m-1}$  and  $t_{m,j}$

$G_i^m$  = volumetric heat capacity weight

=  $C_{p,i}^m HVR_i$  for  $i = 1$

=  $C_{p,i-1}^m HVL_i + C_{p,i}^m HVR_i$  for  $i = 2, \dots, N-1$

=  $C_{p,i-1}^m HVL_i$  for  $i = N$

$C_{p,i}^m$  = volumetric heat capacity of mesh interval  $i$  at time  $t_m$ ,  $J/m^3 \cdot K$

$T_i^m$  = temperature of node  $i$  at time  $t_m$ , K

$T_i^{m-1}$  = temperature of node  $i$  at time  $t_{m-1}$ , K

$m_{film,L}^m$  = mass of film on left boundary surface, kg

$h_{film,L}^m$  = specific enthalpy of film on left boundary surface, kg

$m_{film,R}^m$  = mass of film on right boundary surface, kg

$h_{film,R}^m$  = specific enthalpy of film on right boundary surface, kg

$m$  = denotes quantity of time  $t_m$

$m+1$  = denotes quantity at time  $t_m + \Delta t_m$

## 2.10 Degassing Model

The HS package degassing model assumes that the gas release occurs uniformly over the degassing temperature range. The contribution to the degassing rate for each mesh interval whose temperature exceeds the previously attained maximum is the product of the

source density, volume of the mesh interval, and the fraction of the degassing temperature range that the present maximum represents. Therefore,

$$g_k^m = \sum f \rho_{gas} (HVL + HVR) \frac{(T_2 - T_1)}{(T_{DGmax} - T_{DGmin})} / \Delta t_m \quad (2.130)$$

where

$g_k^m$	= degassing rate for $k$ -th source at time $t_m$ , kg/s
$\sum$	= sum over all heat structure nodes containing gas sources
$f$	= geometry factor
	= surface area of heat structure for rectangular geometries, $m^2$
	= axial length of heat structure for cylindrical geometries, m
	= 1.0 for spherical or hemispherical geometries
$\rho_{gas}$	= source density, $kg/m^3$
$HVL$	= volume weight for left surface (Table 2.1 and Table 2.2)
$HVR$	= volume weight for right surface (Table 2.1 and Table 2.2)
$T_2$	= $\min (T_{nmax}^m, T_{DGmax})$ , K
$T_1$	= $\min (T_{nmax}^{m-1}, T_{DGmax})$ , K
$T_{nmax}^m$	= maximum temperature in mesh interval $n$ at time $t_m$ , K
$T_{nmax}^{m-1}$	= maximum temperature in mesh interval $n$ at time $t_{m-1}$ , K
$T_{DGmax}$	= upper temperature in degassing temperature range, K
$T_{DGmin}$	= lower temperature in degassing temperature range, K
$\Delta t_m$	= system timestep size ( $t_m - t_{m-1}$ ), s

The HS package calculates the mass and internal energy of the gas (at the boundary volume temperature) which is released by each source through the present computational

cycle. These data are then used to update the mass and energy transfer communication arrays for the CVH package.

## 2.11 Ice Condenser Model

The ice condenser model allows the description of certain features found in Westinghouse PWR ice condenser containments. This model is a specially modified application of the heat structure degassing model described in Section 2.10. The user activates the ice condenser logic by including a prescribed keyword in the input for multiple solid, vertical cylindrical structures. A special gas source is defined to release liquid water into the pool of the outer associated CVH volume. The degassing temperature range should have a lower temperature of 274 K to avoid problems associated with limits of the thermodynamic and material properties routines. The upper temperature of the degassing range should be the saturation temperature to account for the sensible heating of the melt water. The heat of reaction of the gas source should include sensible heating of the ice from its actual subcooled temperature to the melting point, the latent heat of fusion, and the sensible heat addition to the melt water from melt to the upper value of the specified degassing temperature range. A special ice condenser Nusselt number multiplier has been added to the gas source input to account for effects not explicitly modeled that may affect the rate of heat transfer to the ice cylinder. Similarly, an ice condenser radionuclide deposition surface area enhancement factor has been added to account for unmodeled effects that will enhance the rate of radionuclide deposition on the ice condenser. Finally, a parameter has been added that can be adjusted by user input to vary the rate of decrease of the ice surface area as the ice melts. The ice surface area will vary as

$$(V/V_o)^{EXPICE}$$

where

$V$  = current ice volume

$V_o$  = initial ice volume

$EXPICE$  = user-specified exponent

The total surface area for heat transfer to the ice condenser (ice and baskets) is the initial surface area of the cylindrical ice columns,  $A_o$ , multiplied by the factor

$$\left[ RNDICE + (1 - RNDICE) \cdot (V/V_o)^{EXPICE} \right]$$

to provide a smooth transition to the minimum surface area of the ice baskets,  $RNDICE \times A_o$ , where  $RNDICE$  is user defined. The total surface area for RN deposition is equal to the ice surface area plus the surface area of the ice baskets. The “gas” source density is that of liquid water.

MELCOR will automatically account for the volume change associated with the reduction in ice mass as melting proceeds. The user should define tabular input to specify properties for the metal baskets that hold the granular ice. The appropriate density is the value of the metal mass divided by the total volume occupied by the baskets. The thermal conductivity should exceed the value associated with ice to account for steam penetration into the granular matrix and conduction in the metal. The specified heat capacity is that of the metal.

## 2.12 Steel Melt Model

To allow for core boundary structure heating and subsequent melting, an option has been included in the degassing model to allow the user to input stainless steel as a degassing source. This option has been included only for use when the COR package is being used and is ignored otherwise. The implementation of the stainless steel degassing source is very similar to that used for ice as part of the ice condenser model (described above) except the heat of reaction of the stainless steel gas source should only include the latent heat of fusion. Because stainless steel is not a hydrodynamic material included in the CVH package, the volume of the melting stainless steel is associated with the COR package materials. As such, these materials are represented by the CVH package as “virtual volume” and, as with the ice condenser model, the volume changes due to melting are explicitly represented.

To prevent potential problems of adding a large amount of heat to a stainless steel degassing structure with an insignificant residual mass, a sensitivity coefficient, 4205, has been provided as a lower limit such that if the remaining unmelted structure mass falls below this limit, then the structure is assumed to have completely melted. When the structure is calculated to have completely melted, it is deactivated and HS processing for this structure is discontinued.

## 2.13 Communication with Other Packages

After completing the calculations discussed in Sections 2.1 through 2.12, the HS package communicates various changes to other packages using well-defined communication interfaces. The HS package communicates to the CVH package any mass, energy, and virtual volume changes in each control volume due to the following mechanisms:

- (1) heat transfer between each heat structure and the pool and atmosphere of its boundary volumes

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- (2) condensation of steam onto each heat structure from the atmosphere of its boundary volumes
- (3) evaporation or flashing of liquid (water) from each heat structure boundary surface into the atmosphere of its boundary volumes
- (4) deposition of liquid (water) from each heat structure into the pool of its boundary volumes
- (5) degassing of materials within each heat structure

The virtual volume with which the HS package is concerned is the volume occupied by all water films, ice condenser ice and meltable (degassible) steel associated with the core boundary structure melting model. Initial values of virtual volume are calculated during MELGEN execution and changes in virtual volume are calculated each computational cycle during MELCOR execution.

Prior to communication of control volume mass and energy changes to the CVH package, the HS package determines if these changes will lead to a negative mass of some material. If a negative mass is detected, the HS package requests that the present computational cycle be repeated with a timestep reduction and the changes not be communicated to the CVH package.

During MELCOR execution, the HS package calculates and communicates to the RadioNuclide (RN) package the fraction of liquid (water) mass on each heat structure boundary surface deposited during each computational cycle in the pool of its boundary volume. These fractions are used to calculate the relocation of radionuclides from deposition surfaces to the pools of their boundary volumes.

### 3. Solution Methods

The finite-difference approximation to the heat conduction equation with boundary conditions utilized by the HS package results in a tridiagonal system of  $N$  equations ( $N+1$  or  $N+2$  if there is a liquid film on one or both surfaces) for a heat structure with  $N$  ( $N+1$  or  $N+2$ ) temperature nodes. In order to reduce roundoff problems, the temperature of the heat structure relative to the minimum value of that heat structure is used to set up and solve the equations. The solution procedure is usually more complex than the standard solution for a tridiagonal system of equations. The boundary conditions often include energy input due to mass transfer and may include the deposition of energy from other sources such as decay-heat of radionuclides. Furthermore, the temperature nodes near the surface of a heat structure may be too closely spaced to accurately calculate the temperature at the surface, or the computational timestep may be large. This section discusses some of the special solution procedures that are used to obtain the steady-state and transient temperature distribution of a heat structure.



### 3.1 Iteration Strategy

By default an iterative procedure is employed to determine the temperature profile in each heat structure. This procedure repeats the following calculations until either convergence is attained or a maximum number of iterations is performed:

- (1) thermal properties
- (2) heat transfer coefficients
- (3) mass transfer
- (4) boundary condition coefficients
- (5) temperature distribution

Convergence is determined by testing the relative error in several dependent variables calculated during the temperature iteration:

- (1) the temperature at each node in the structure (including the film interfacial temperature[s]),
- (2) the mass of the film(s) (if the film thickness exceeds  $10^{-5}$  m), and
- (3) the boiling heat transfer coefficient(s).

The relative error for dependent variable  $X$  is defined as

$$ERR_X = (X^m / X^{m-1}) - 1 \quad (3.1)$$

where

$X^{m-1}$  = value of  $X$  at iteration  $m-1$

$X^m$  = value of  $X$  at iteration  $m$

If the relative error in the temperature profile falls below a threshold value ( $ERR_{prp}$  in Section 3.3 below) during an iteration, then material properties are generally not recalculated for that iteration step. Values from the previous iteration step are used until the relative error again becomes higher than  $ERR_{prp}$  or until convergence is achieved. However, during degassing, properties must be updated after every iteration to ensure sufficient accuracy of the degassing rate.

Relaxation of the pool boiling heat transfer coefficient may be required in some situations, since it is extremely sensitive to changes in the surface temperature. Because relaxation

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effectively falsifies the value of the heat transfer coefficient until the relaxed value stabilizes, it is necessary to check the relative difference (error) between the unrelaxed value (which is determined by the latest surface temperature iterate) and the relaxed value. When pool boiling occurs, the pool heat transfer coefficient  $h_{pool}^m$  is relaxed between temperature iterations to be:

$$W_B h_{pool}^m + (1 - W_B) h_{pool}^{m-1}$$

where

$$h_{pool}^{m-1} = \text{pool heat transfer coefficient at iteration } m-1, \text{ W/m}^2\cdot\text{K}$$

$$h_{pool}^m = \text{pool heat transfer coefficient at iteration } m, \text{ W/m}^2\cdot\text{K}$$

and  $W_B$  is the modified relaxation parameter, which is set to an initial value that depends on whether it is a steady-state or transient iteration ( $RLX_B$  in Sections 3.2 and 3.3 below), and which is then decreased by a factor of 0.95 for each iteration during which the relative error in the boiling surface temperature is greater than -0.5 (i.e., the boiling surface temperature is not oscillating excessively so that relaxation may be reduced).

The system of equations describing the transient temperatures within a structure can become ill-conditioned if the timestep becomes too large. A precision limit ( $P_{illmat}$  in Section 3.3) is imposed in the routine that performs the direct inversion of the tridiagonal coefficient matrix. If the relative difference between terms used in evaluating a nonzero difference in the algorithm is less than this limit, then there are too few significant figures in the difference to achieve the requested degree of precision. During MELGEN execution this condition is fatal but may be corrected by reducing the value of  $\Delta t_o$ , discussed in Section 3.2 below. During MELCOR execution the cycle will be repeated with a smaller timestep in an attempt to alleviate the problem.

There are three levels of convergence criteria used: the desired convergence criteria, a more stringent override convergence criterion, and the less stringent acceptance convergence criteria. The desired and acceptance criteria may be assigned different values for MELGEN and MELCOR execution, as discussed in Sections 3.2 and 3.3, respectively.

The desired convergence criteria are normally stringent enough to ensure reasonable accuracy in the overall results in the absence of phenomena that demand very high temperature resolution. During the occurrence of phenomena such as degassing or mass transfer (condensation/evaporation), however, very small errors in temperature can cause quite large errors in degassing and mass transfer rates. Therefore, during the occurrence of degassing or mass transfer, the desired temperature convergence criteria are overridden

by the override temperature convergence criterion (as long as it is more stringent). The override temperature convergence criterion is contained in sensitivity coefficient array 4055 and discussed in Section 3.3 below.

The iteration procedure for a heat structure will continue until either the desired criteria (or the override criterion during degassing or mass transfer) have been met or the iteration count reaches a prescribed maximum. During override, convergence is declared after the maximum number of iterations if the desired criteria have been met, even though the more stringent criterion has not been satisfied. If the acceptance criteria have not been satisfied for all tested variables on a heat structure after the maximum number of permitted iterations is performed, failure is declared for that heat structure. If the acceptance criteria have been met but the desired criteria have not been met, then success is declared but a message is issued to warn the user that the desired criteria were not met.

### 3.2 Steady-State Convergence Criteria

During MELGEN execution, an initial temperature distribution is calculated for a given heat structure if specified by user input. The following constants are the iteration parameters used for steady-state heat conduction calculations. They are implemented as sensitivity coefficient array C4051.

$ITR_{ss}$  = maximum number of permitted steady-state iterations (default = 400)

$ERR_{ss}$  = desired relative error tolerance for temperatures during steady-state calculations (default =  $10^{-5}$ )

$\Delta t_o$  = initial steady-state timestep (default =  $10^5$  s)

$ERF_{ss}$  = desired relative error tolerance for film mass for steady-state calculations (default =  $10^{-2}$ )

$DIE_{ss}$  = acceptable relative error tolerance for temperature during steady-state calculations (default =  $10^{-2}$ )

There is no acceptance criterion for film mass; the iteration procedure will continue for  $ITR_{ss}$  iterations in an attempt to satisfy the desired criterion,  $ERF_{ss}$ , but after  $ITR_{ss}$  iterations the film mass value is declared acceptable no matter what. The following coefficients are the iteration relaxation parameters used for steady-state heat conduction calculations to mitigate temperature oscillations. They are implemented as sensitivity coefficient array C4052.

$RLX_B$  = steady-state boiling heat transfer coefficient relaxation parameter (default = 0.0)

$ERR_B$  = desired steady-state boiling heat transfer coefficient error tolerance (default = 0.05)

The boiling heat transfer coefficient relative error acceptance criterion is 100%, that is it may double or vanish.

If any heat structure fails to meet the acceptance criteria, a restart file is not written and MELCOR execution may not begin.

### 3.3 Transient Convergence Criteria

During MELCOR execution, an iterative procedure is invoked if specified by user input (highly recommended). The following constants are the iteration parameters used for transient heat conduction calculations. They are implemented as sensitivity coefficient array C4055.

$ITR_{trn}$  = maximum number of transient iterations (default = 30.)

$ERR_{trn}$  = desired relative error tolerance for temperature during transient conduction calculations (default = 0.0005)

$ITR_{cut}$  = minimum number of transient iterations required to prevent increase of the timestep size (default = 31.)

$ERR_{prp}$  = minimum relative error tolerance for material property determination (default = 0.01)

$P_{illmat}$  = tridiagonal matrix solver precision requirement (default =  $1.0 \times 10^{-10}$ )

$ERR_{ovr}$  = error tolerance override during degassing/mass transfer (default =  $5.0 \times 10^{-6}$ )

$ERF_{trn}$  = maximum relative error tolerance for film mass during transient conduction calculations (default = 0.01)

$DIE_{trn}$  = maximum relative error tolerance for transient temperature during conduction calculations (default = 0.005)

There is no acceptance criterion for film mass; the iteration procedure will continue for  $ITR_{trn}$  in an attempt to satisfy the desired criterion,  $ERF_{trn}$ , but after  $ITR_{trn}$  iterations the film mass value is declared acceptable no matter what. The boiling heat transfer coefficient relative error acceptance criterion is 100%, that is, it may double or vanish.

Although inactive by default, the value of  $ITR_{cut}$  can be adjusted downward (below  $ITR_{trn}$ ) to prevent the MELCOR system timestep from increasing if the HS package is taking too

many iterations per timestep. Judicious use of this feature requires comparing total CPU usage for various strategies.

The following constants are the relaxation parameters used for transient calculations. These parameters are implemented as sensitivity coefficient array C4056:

$RLX_B$  = transient boiling heat transfer coefficient relaxation parameters (default = 0.9)

$ERR_T$  = transient boiling heat transfer coefficient error tolerance (default = 0.05)

If the temperature solution fails for any structure during a calculation cycle, the HS package will immediately request that the cycle be repeated with the timestep reduced by a factor of one half. Failure may occur for several reasons, including excessive error in the temperatures, excessive error in the boiling heat transfer coefficient, numerical problems associated with finite precision or the generation of an out-of-range temperature (less than 273 K or greater than 4990 K), either legitimately or from divergence of the iterative algorithm.

#### 4. Timestep Control

Timestep control is exercised by the Heat Structure package in cases (a) and (b) below by the HS package requesting that the current timestep be repeated with a smaller timestep size to correct the problem.

- (a) condensation is causing excessive steam depletion in the CVH package as discussed in Section 2.7.3 or,
- (b) the temperature solution for a heat structure fails to converge within the prescribed maximum number of iterations as discussed in Section 3.3. (a timestep reduction request to one-half the current timestep will also be made if a physically unreasonable value is detected during the iterative solution).

In these cases, the HS package will request that the current timestep be repeated with a smaller timestep size to attempt to correct the problem.

## APPENDIX A: Sensitivity Coefficients

This appendix provides the sensitivity coefficients associated with various correlations and modeling parameters used in the HS package and described in this reference manual.

Equation or Section	Coefficient	Value	Units
(2.109)	C4000(1)	0.2358	N/m
	C4000(2)	1.0	
	C4000(3)	-0.625	K <sup>-1</sup>
	C4000(4)	1.256	
	C4000(5)	0.	N/m
	C4000(6)	1.0	
	C4000(7)	647.3	K
Section 3.2	C4051(1)	400.	
	C4051(2)	10 <sup>-5</sup>	
	C4051(3)	10 <sup>5</sup>	s
	C4051(4)	0.01	
	C4051(5)	0.01	
Section 3.2	C4052(1)	0.0	
	C4052(2)	0.05	
Section 3.3	C4055(1)	30.	
	C4055(2)	0.0005	
	C4055(3)	31.	
	C4055(4)	0.01	
	C4055(5)	10 <sup>-10</sup>	
	C4055(6)	5.x10 <sup>-6</sup>	
	C4055(7)	0.01	
	C4055(8)	0.005	
Section 3.3	C4056(1)	0.9	
	C4056(2)	0.05	
(2.79) - (2.81)	C4060(1)	1.0	
	C4060(2)	10.0	
(2.85) - (2.87)	C4061(1)	10 <sup>9</sup>	
	C4061(2)	10 <sup>10</sup>	
	C4062(1)	10 <sup>9</sup>	
	C4062(2)	10 <sup>10</sup>	
	C4063(1)	10 <sup>9</sup>	
	C4063(2)	10 <sup>10</sup>	
(2.88a)–(2.90b)	C4064(1)	3.0x10 <sup>5</sup>	
	C4064(2)	6.0x10 <sup>5</sup>	
	C4065(1)	2.0x10 <sup>3</sup>	

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Equation or Section	Coefficient	Value	Units
	C4065(2)	$10^4$	
	C4066(1)	$2.0 \times 10^3$	
	C4066(2)	$10^4$	
(2.4)	C4071(1)	0.02	
	C4071(2)	0.98	
(2.97) - (2.99)	C4080(1)	1.0	
	C4080(2)	10.0	
(2.102) - (2.104)	C4081(1)	$10^9$	
	C4081(2)	$10^{10}$	
	C4082(1)	$10^9$	
	C4082(2)	$10^{10}$	
	C4083(1)	$10^9$	
	C4083(2)	$10^{10}$	
(2.105) – (2.107)	C4084(1)	$3.0 \times 10^5$	
	C4084(2)	$6.0 \times 10^5$	
	C4085(1)	$2.0 \times 10^3$	
	C4085(2)	$10^4$	
	C4086(1)	$2.0 \times 10^3$	
	C4086(2)	$10^4$	
(2.82)	C4101(1)	0.046	
	C4101(2)	1/3	
	C4101(3)	0.	
(2.82)	C4102(1)	0.046	
	C4102(2)	1/3	
	C4102(3)	0.	
(2.82)	C4103(1)	0.228	
	C4103(2)	0.226	
	C4103(3)	0.	
(2.82)	C4104(1)	0.046	
	C4104(2)	1/3	
	C4104(3)	0.	
(2.82)	C4105(1)	0.046	
	C4105(2)	1/3	
	C4105(3)	0.	
(2.82)	C4106(1)	0.228	
	C4106(2)	0.226	
	C4106(3)	0.	
(2.82)	C4107(1)	0.59	
	C4107(2)	0.25	
	C4107(3)	0.	

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Equation or Section	Coefficient	Value	Units
(2.82)	C4108(1)	0.59	
	C4108(2)	0.25	
	C4108(3)	0.	
(2.82)	C4109(1)	0.43	
	C4109(2)	0.25	
	C4109(3)	12.0	
(2.82)	C4110(1)	0.10	
	C4110(2)	1/3	
	C4110(3)	0.	
(2.82)	C4111(1)	0.10	
	C4111(2)	1/3	
	C4111(3)	0.	
(2.82)	C4112(1)	0.43	
	C4112(2)	0.25	
	C4112(3)	2.0	
(2.83)	C4113(1)	8.235	
	C4113(2)	0.	
	C4113(3)	0.	
	C4113(4)	0.	
(2.83)	C4114(1)	48/11	
	C4114(2)	0.	
	C4114(3)	0.	
	C4114(4)	0.	
(2.83)	C4115(1)	48/11	
	C4115(2)	0.	
	C4115(3)	0.	
	C4115(4)	0.	
(2.83)	C4116(1)	0.023	
	C4116(2)	0.8	
	C4116(3)	1/3	
	C4116(4)	0.	
(2.83)	C4117(1)	0.023	
	C4117(2)	0.8	
	C4117(3)	1/3	
	C4117(4)	0.	
(2.83)	C4118(1)	0.023	
	C4118(2)	0.8	
	C4118(3)	1/3	
	C4118(4)	0.	
(2.83)	C4119(1)	0.664	



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Equation or Section	Coefficient	Value	Units
	C4119(2)	0.5	
	C4119(3)	1/3	
	C4119(4)	0.	
(2.83)	C4120(1)	0.664	
	C4120(2)	0.5	
	C4120(3)	1/3	
	C4120(4)	0	
(2.83)	C4121(1)	0.60	
	C4121(2)	0.5	
	C4121(3)	1/3	
	C4121(4)	2.0	
(2.83)	C4122(1)	0.037	
	C4122(2)	0.8	
	C4122(3)	1/3	
	C4122(4)	0.	
(2.83)	C4123(1)	0.037	
	C4123(2)	0.8	
	C4123(3)	1/3	
	C4123(4)	0.	
(2.83)	C4124(1)	0.60	
	C4124(2)	0.5	
	C4124(3)	1/3	
	C4124(4)	2.0	
(2.100)	C4151(1)	0.046	
	C4151(2)	1/3	
	C4151(3)	0.	
(2.100)	C4152(1)	0.046	
	C4152(2)	1/3	
	C4152(3)	0.	
(2.100)	C4153(1)	0.228	
	C4153(2)	0.226	
	C4153(3)	0.	
(2.100)	C4154(1)	0.046	
	C4154(2)	1/3	
	C4154(3)	0.	
(2.100)	C4155(1)	0.046	
	C4155(2)	1/3	
	C4155(3)	0.	
(2.100)	C4156(1)	0.228	
	C4156(2)	0.226	

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Equation or Section	Coefficient	Value	Units
	C4156(3)	0.	
(2.100)	C4157(1)	0.59	
	C4157(2)	0.25	
	C4157(3)	0.	
(2.100)	C4158(1)	0.59	
	C4158(2)	0.25	
	C4158(3)	0.	
(2.100)	C4159(1)	0.43	
	C4159(2)	0.25	
	C4159(3)	2.0	
(2.100)	C4160(1)	0.10	
	C4160(2)	1/3	
	C4160(3)	0.	
(2.100)	C4161(1)	0.10	
	C4161(2)	1/3	
	C4161(3)	0.	
(2.100)	C4162(1)	0.43	
	C4162(2)	0.25	
	C4162(3)	2.0	
(2.101)	C4163(1)	8.235	
	C4163(2)	0.	
	C4163(3)	0.	
	C4163(4)	0.	
(2.101)	C4164(1)	48/11	
	C4164(2)	0.	
	C4164(3)	0.	
	C4164(4)	0.	
(2.101)	C4165(1)	48/11	
	C4165(2)	0.	
	C4165(3)	0.	
	C4165(4)	0.	
(2.101)	C4166(1)	0.023	
	C4166(2)	0.8	
	C4166(3)	1/3	
	C4166(4)	0.	
(2.101)	C4167(1)	0.023	
	C4167(2)	0.8	
	C4167(3)	1/3	
	C4167(4)	0.	
(2.101)	C4168(1)	0.023	

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Equation or Section	Coefficient	Value	Units
	C4168(2)	0.8	
	C4168(3)	1/3	
	C4168(4)	0.	
(2.101)	C4169(1)	0.664	
	C4169(2)	0.5	
	C4169(3)	1/3	
	C4169(4)	0.	
(2.101)	C4170(1)	0.664	
	C4170(2)	0.5	
	C4170(3)	1/3	
	C4170(4)	0.	
(2.101)	C4171(1)	0.60	
	C4171(2)	0.5	
	C4171(3)	1/3	
	C4171(4)	2.0	
(2.101)	C4172(1)	0.037	
	C4172(2)	0.8	
	C4172(3)	1/3	
	C4172(4)	0.	
(2.101)	C4173(1)	0.037	
	C4173(2)	0.8	
	C4173(3)	1/3	
	C4173(4)	0.	
(2.101)	C4174(1)	0.60	
	C4174(2)	0.5	
	C4174(3)	1/3	
	C4174(4)	2.0	
(2.108)	C4180(1)	0.013	
	C4180(2)	0.5	
	C4180(3)	1.0	
	C4180(4)	0.33	
(2.110)	C4181(1)	0.18	
	C4181(2)	0.25	
	C4181(3)	0.5	
(2.111)	C4182(1)	0.09	
	C4182(2)	0.25	
	C4182(3)	0.5	
(2.112)	C4183(1)	0.943	
	C4183(2)	0.25	
	C4183(3)	0.75	

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Equation or Section	Coefficient	Value	Units
(2.116)	C4184(1)	0.943	
Section 2.7	C4200(1)	0.9995	
(2.119)	C4201(1)	1.0	
	C4201(2)	1.0	
	C4201(3)	1/3	
	C4201(4)	-1/3	
(2.122)	C4202(1)	$5 \times 10^5$	W/m <sup>2</sup> -K
Section 2.7.3	C4203(1)	-1.0	
	C4203(2)	0.9	
Section 2.12	C4205(1)	10.	kg
Section 2.6.1.1	C4210(1)	30.	
	C4210(2)	100.	
	C4210(3)	(not used)	
	C4210(4)	0.1686289	
Section 2.6.1.1	C4211(1)	0.943	
	C4211(2)	0.25	
Section 2.6.1.1	C4212(1)	0.3333333	
	C4212(2)	-0.44	
	C4212(3)	$5.82 \times 10^{-6}$	
	C4212(4)	0.8	
	C4212(5)	0.3333333	
	C4212(6)	0.5	
Section 2.6.1.1	C4213(1)	$10^6$	
	C4213(2)	$10^8$	
	C4213(3)	$10^{10}$	
Section 2.6.1.1	C4214(1)	0.6	
	C4214(2)	0.2	
Section 2.6.1.1	C4215(1)	0.72	
	C4215(2)	0.19	
Section 2.6.1.1	C4220(1)	30.	
	C4220(2)	100.	
	C4220(4)	0.9715642	
Section 2.6.1.1	C4221(1)	0.729	
	C4221(2)	0.25	
Section 2.6.1.1	C4222(1)	0.3333333	
	C4222(2)	-0.44	
	C4222(3)	$5.82 \times 10^{-6}$	
	C4222(4)	0.8	
	C4222(5)	0.3333333	
	C4222(6)	0.5	

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Equation or Section	Coefficient	Value	Units
Section 2.6.1.1	C4230(1)	30.	
	C4230(2)	100.	
Section 2.6.1.1	C4231(1)	0.815	
	C4231(2)	0.25	
Section 2.6.1.1	C4232(1)	0.3333333	
	C4232(2)	-0.44	
	C4232(3)	$5.82 \times 10^{-6}$	
Section 2.6.1.1	C4232(4)	0.8	
	C4232(5)	.3333333	
	C4232(6)	0.5	
Section 2.8.1	C4251(1)	$10^{-9}$	
Section 2.8.2	C4251(2)	0.0005	
Sections 2.6.1.2 & 2.8.2	C4253(1)	0.909	
	C4253(2)	0.3333333	
	C4253(3)	0.115	
	C4253(4)	0.6	
	C4253(5)	1000.	
	C4253(6)	3000.	
	C4253(7)	-0.44	
	C4253(8)	$5.82 \times 10^{-6}$	
	C4253(9)	0.8	
	C4253(10)	0.3333333	
	C4253(11)	0.5	

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